⁵⁶Fe Evaluation in the Fast Neutron Region

D. Brown, M. Herman, S. Hoblit, G.P.A. Nobre, E. McCutchan (BNL) Jing Qian, Zhigang GE, Tingjin LIU, Xichao Ruan, Zuying ZHOU (CNDC) V. Pronyaev (IPPE) S. Tagesen, H. Vonach (IRK, Vienna) R. Capote, A. Trkov (IAEA) A. Plompen (IRMM) G. Zerovnik (JSI)



a passion for discovery



- GForge CIELO-Iron project set up and contains lot of information
 - previous evaluations
 - new resonance region evaluation by L. Leal (ORNL)
 - EMPIRE inputs and calculations (future new evaluation) (NNDC)
 - some historic documents and recent publications/presentations
 - selection of relevant integral experiments (G. Zerovnik, JSI)
- Empire updated to natively produce CN angular distributions (elastic and inelastic)
- New non-linear fitting (differential and/or integral data) in EMPIRE
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- Guided by Zolotarev IRDF-2002 file for ⁵⁶Fe(n,p)
- Preliminary calculations adjusted to differential data look good!



Along the way we have:

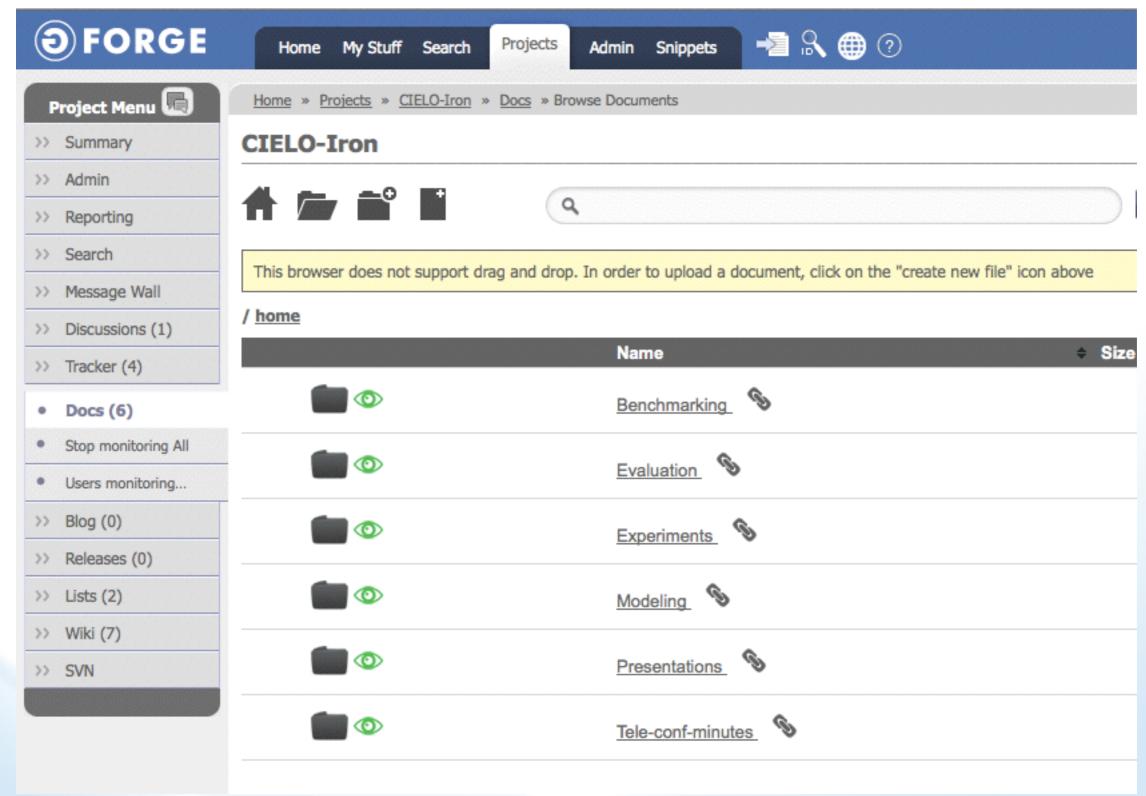
- solved mystery in the ENSDF/RIPL 56Fe level scheme
- discovered extraordinary sensitive monitor of level densities
- rediscovered Toshihiko's finding that OM for ⁵⁶Fe fails below 3
 MeV
- got a suspicion that angular distributions might be the key to the good iron evaluation
- realized the importance of having clean, differential data based, evaluation for being able to perform future updates



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GForge CIELO-Iron project



GForge CIELO-Iron - evaluation docs

Chien-resonance-evaluation.pdf	199.82 KB	application/pdf
effdoc-085Vonach 91.pdf	6.84 MB	application/pdf
effdoc-184Vonach 92.pdf	4.9 MB	application/pdf
effdoc-378Pronyaev 94.pdf	4.52 MB	application/pdf
Froehner-reevaluation.pdf	244.42 KB	application/pdf
Froehner-Resonance-parameters-fluctuations-evaluation.pdf	684.84 KB	application/pdf
IRDF-2002.pdf	3.17 MB	application/pdf
McGNASH-calculations.pdf	135.79 KB	application/pdf
Moxon-evaluation-58Fe-RR.pdf	1.16 MB	application/pdf
NDS-vol118-p001-CIELO-paper.pdf	304.47 KB	application/pdf
UNF-calc-for-iron-isotopes.ppt	5.86 MB	application/vnd.ms- powerpoint
WPEC-SG2-evaluation.pdf	109.9 KB	application/pdf
Zolotarev-54Fe-np-IRDF.pdf	660.87 KB	application/pdf

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GForge CIELO-Iron evaluation

Index of /trunk/CIELO-EVAL

Edit permissions for this directory

Files shown: 1

Directory revision: 34 (of 34)

Sticky Revision:

Set

<u>File</u> ▲	Rev.	Age	<u>Author</u>	Last log entry
Parent Directory				
Fast/	34	28 hours	gnobre	Removed spurious first 3- state (level index #7) from collective level file.
Resonances/	11	6 months	dbrown	Luiz's 56Fe RRR starter files + fixes
README.txt	12	6 months	dbrown	a readme

Index of /trunk/CIELO-EVAL/Fast

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Files shown: 18

Directory revision: 34 (of 34)

Sticky Revision:

Set

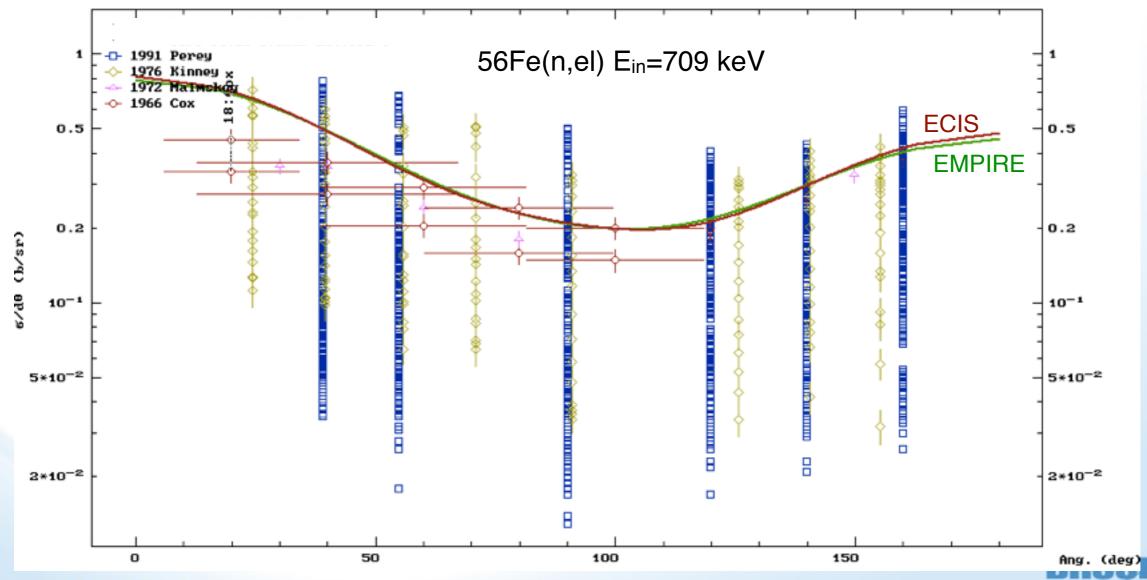
<u>File</u> ▲	Rev.	Age	<u>Author</u>	Last log entry
Parent Directory				
CIELO-Iron-lev.col	34	28 hours	gnobre	Removed spurious first 3- state (level index #7) from collective level file.
CIELO-Iron-omp.dir	14	6 months	gnobre	Preliminary input and outfiles for the new 56Fe evaluation for the CIELO calcula
CIELO-Iron-omp.ripl	27	3 weeks	gnobre	New input and outputs, obtained with Rev. 4130 of EMPIRE. It has a cleaner input
CIELO-Iron.c4	28	6 days	gnobre New inputs and outputs. Calculation was done using Rev.4158 of EMPIRE with	
☐ CIELO-Iron.endf	34	28 hours	gnobre	Removed spurious first 3- state (level index #7) from collective level file.
CIELO-Iron.inp	29	5 days	gnobre	Corrected the (n,p) cross section by fitting 56Mn level-density parameters ROHFB
<u> CIELO-Iron.lev</u>	14	6 months	gnobre	Preliminary input and outfiles for the new 56Fe evaluation for the CIELO calcula
<u> CIELO-Iron.lst</u>	34	28 hours	gnobre	Removed spurious first 3- state (level index #7) from collective level file.
OMINATEL SCIENCE ASSOCIATES				• *************************************

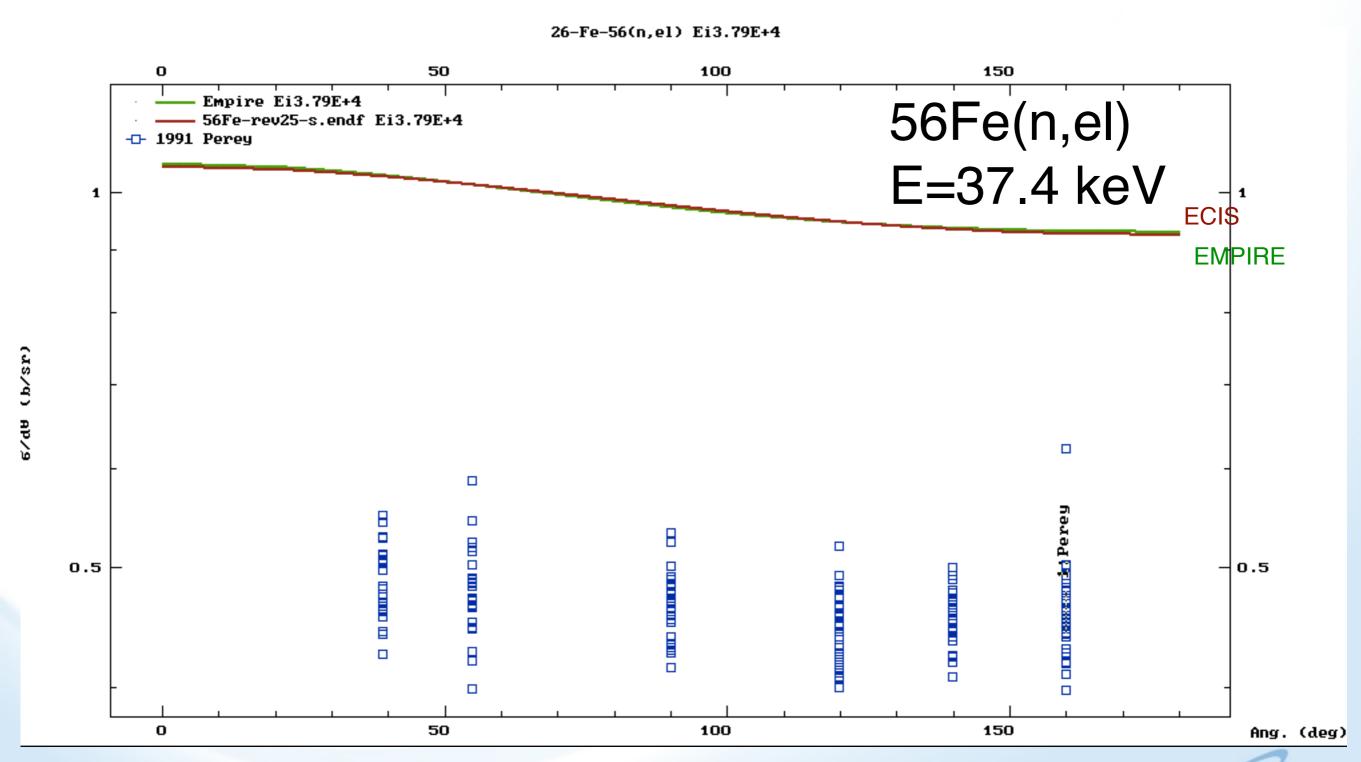
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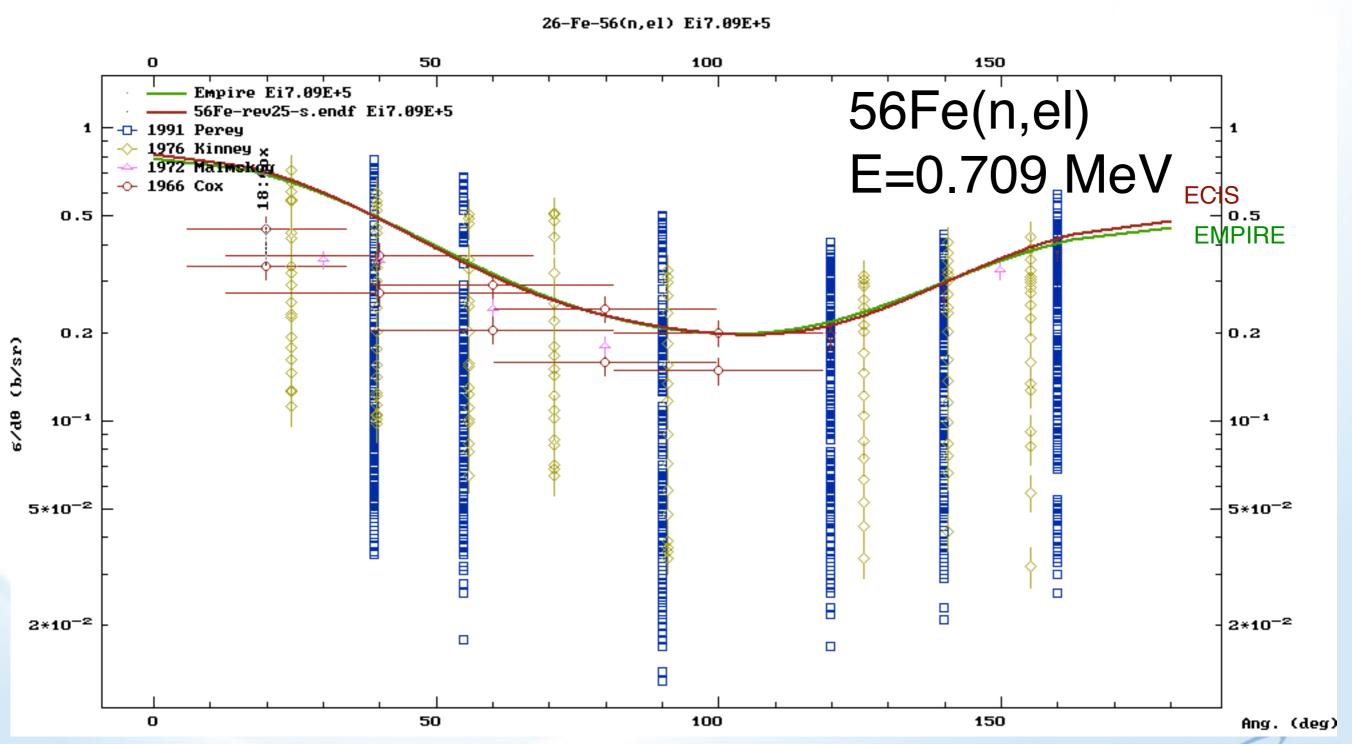


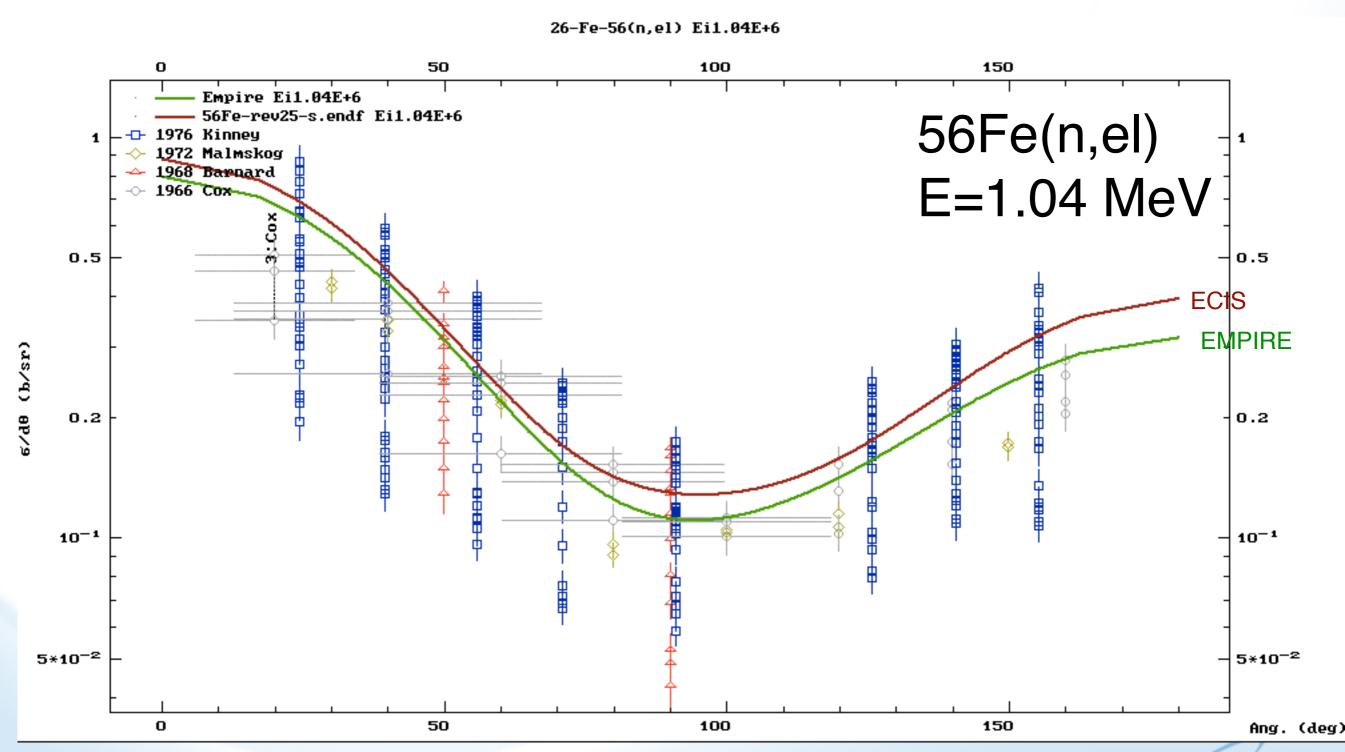
CN angular distributions in EMPIRE

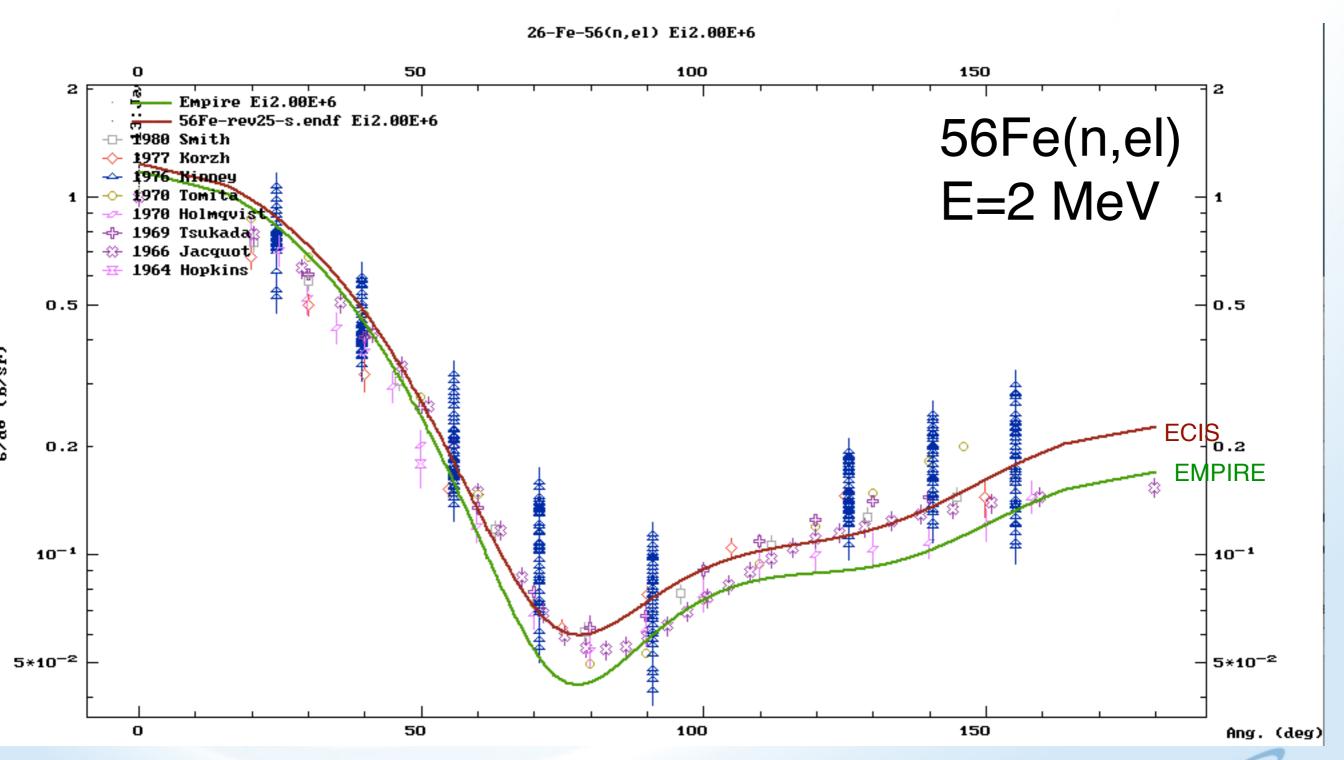
- Previously CN angular distr.
 were calculated by rescaling
 ECIS results not fully
 consistent and cumbersome
- Native EMPIRE calculations required replacing T_I with T_{Ij}
- New HRTW subroutine was totally recoded in F90











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New non-linear fitting in EMPIRE by Sam Hoblit

- Uses surrogate surface instead of actual EMPIRE obtained from sensitivity calculations
- CERN code MINUIT to minimize Chi**2 through variation of model parameters
- Experimental data scaled with a factor (with penalty!) to account for systematic errors BONUS - no PPP
- Differential, integral, and differential+integral data possible

- Great flexibility through line command control
 - ex- in-cluding experiments
 - ex- in-cluding reactions
 - ex- in-cluding parameters
 - freezing parameters
 - freezing scaling factors
 - plotting fits and covariances

Unfortunately Sam got sick before he could use it.



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There is WAY too much data to get through. We needed "a little help from our friends..."

- 56Fe has 447 EXFOR sets with points in the fast region
- natFe (91.72% ⁵⁶Fe)
 has 838 EXFOR sets
 with points in the Fast
 Region



Our CNDC colleagues generated an authoritative review of data & previous evaluations

List of the experimental information for 56Fe

Three evaluated documents of EFF from H.Vonach and V.Pronyaev in 1992 and 1995, they gave a detail experimental data evaluation of the fast neutron cross sections of 56Fe, even including complete covariance info

The report of 1995 was based on a few new experimental data including the total cross section and (n,a) cross section.

It was the updated of the 56Fe evaluation.

After 1995, there are very few experimental data in EXFOR for natural iron and iron 56,so we take these three documents as the reference of our experimental data evaluation.

REF: Evaluated by vonach91/effdoc-085 vonach92/effdoc-184 pronyaev95/effdoc-378

Evaluated data:

ENDF/B-VII.1 JENEL-4.0 ROSFOND JEFF-3.1 JEFF-3.2 CNEDL-2.1 CENDL-3.1 Theortical calculation UNF EAF

Total Cross section

(Because the isotopical dependence of the total cross section for the non-resonance region is rather weak, we used the data of natural iorn for the evaluation of the 56Fe total cross section.)

Data come recommend: ENDF/B-VII.1

Figure shows the evaluated result from different libraries(B71 C31 F31 J40 ROSFOND) and a new theoretical calculated result from CNDC, which used UNF series codes. We can see that the evaluated result from different libraries are consistent in the fast neutron region(above 10MeV). The total cross section in general known with an accuracy of about 1~3%.

ENDF FILE ENDF/B-

VII.1

Selected ExpData

Sheet

(Vonach92)

ExpFigure/

EXPData

(uncorrected)

Exp+EvalFigure

Nonelastic cross section (Acording to Energy and Resource)

The other important reaction is nonelastic cross sections.

The nonelastic cross section for fast neutron energies(E>4MeV in 56Fe) is measured with a higher accurancy than the elastic scattering cross section;

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From this careful review, our friends at the CNDC recommend we build on the work of these fellows; we agree with their recommendation



Siegfried Tagesen



Herbert Vonach



Vladimir Pronyaev



EFF-3.1 contains most complete review of experimental data in the

Fast region

EFF-Doc-184

EFF-DOC-85

Uncertainty Estimates for the Fast Neutron Cross-Sections of the European Fusion File EFF for 52Cr, 56Fe, 58Ni and 60Ni and Evaluation of the 14 MeV Cross-Sections of these Isotopes from the existing experimental data base

FINAL REPORT FOR CONTRACT Nr. 395-89-8/FU-D/NET

H. VONACH,S. TAGESEN, M. WAGNER and A. PAVLIK

EVALUATION OF THE
FAST NEUTRON CROSS SECTIONS
OF 55FE

EFF-Doc-378 (1995)

Evaluations of the fast neutron cross sections of 52Cr and 56Fe including complete covariance information

V. Pronyaev*, S. Tagesen, H. Vonach and S. Badikov*

Institut für Radiumforschung und Kernphysik der Universität Wien, Austria

*) Permanent address: Institute of Physics and Power Engineering, 249020 Obninsk, Kaluga Reg., Russia



Summary of (n,2n) data

<u>Table 11:</u> Experimental data base for the evaluation of the cross section for the $\frac{56\text{Fe}(n,2n)^{55}\text{Fe}}{100}$ reaction.

EXFOR First Author Entry and Year No.	Energy range	No. of	Comments	Corrections	Uncertainties (%)		χ^2	
	and Year	(MeV)	data points		applied	Statistical (uncorrel.)	Systematic (correl.)	per degree of freedom
11097	Ashby 58	14.1	1	neutron detection nat Fe	1) normalization by a factor 0.815	7.8(total)		0.03
20091	Wenusch 62	14.8	1	activ., enriched ⁵⁶ Fe	recent reference cross section	20.5 (total)		0.74
20721	Qaim 76	14.7	1	activ., enriched ⁵⁶ Fe	-	9.1 (total)		1.17
12936	Auchampaugh 80	14.7-20.0	6	neutron detection, nat Fe	2)	4.3-9.5	4	0.31
20416.044	Fréhaut 80A	11.88-14.76	7	neutron det. ^{nat} Fe	renormalization	2.7-17	6.2	1.50 ³⁾
20416.003	Fréhaut 80B	11.88-14.76	7	neutron detection enriched ⁵⁶ Fe	by a factor 1.077	2.6-9.6	5.1	
13132	Greenwood 88	14.8	1	activ., enriched ⁵⁶ Fe	· -	7.7 (total)		0.72

correct. for minor Fe isotopes 1)

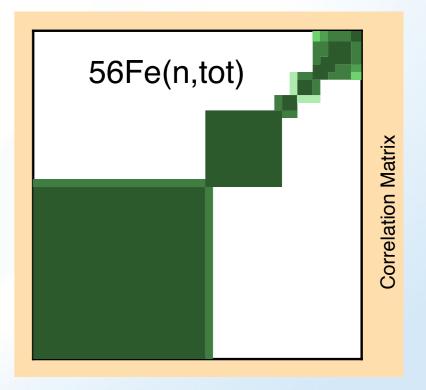
correct. for minor Fe isotopes; correc. for energy-dependent efficiency of the detector (see text)

²⁾ because of strong correlations the results of both experiments were processed as one single data set.

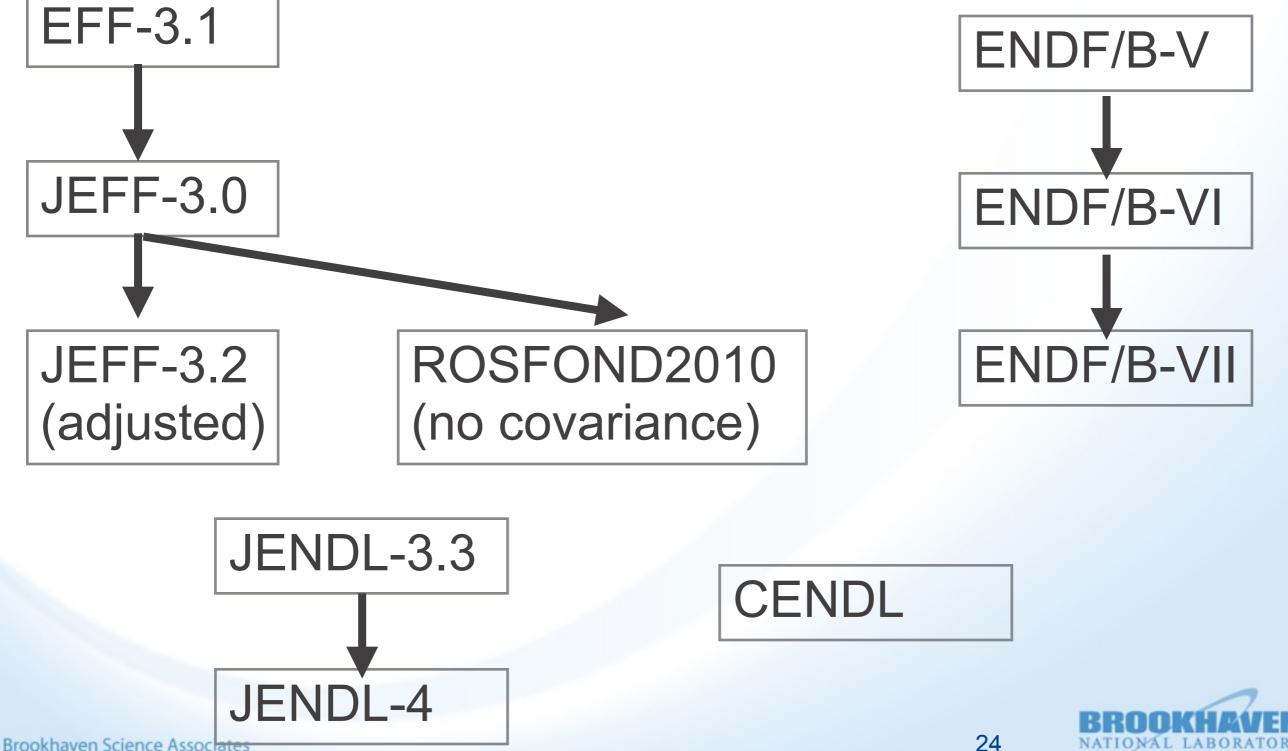
The EFF-3.1 evaluation was a Frankenevaluation, but with good parts

- Constraint LSQR fit using GLUCS of all data for (n,tot), (n,el), (n,γ), (n,inel), (n,n₁¹)-(n,n₄₀²), (n,2n), (n,α), (n,p)
 - Best fit cross sections
 - Cross-reaction covariance
 - Careful assessment of med. & long range correlations
- Update for JEFF-3.0 included (n,tot) data of Weigmann
- Everything else is model based, and kind of wonky
- JEFF-3.2 based on JEFF-3.0, but it was adjusted;



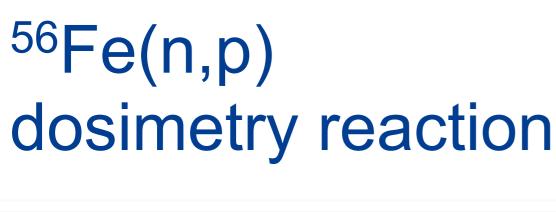


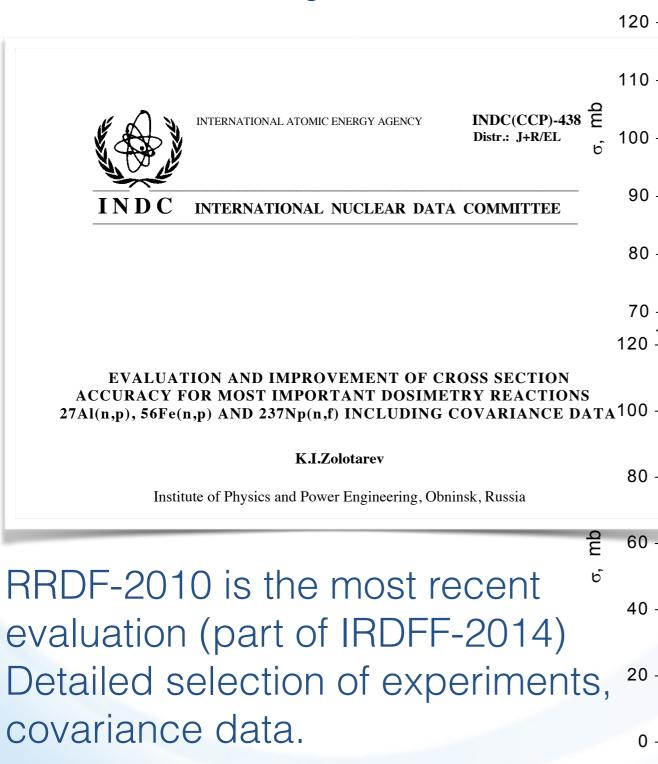
Only EFF-3.1 and JEFF-3.0 contain original evaluation

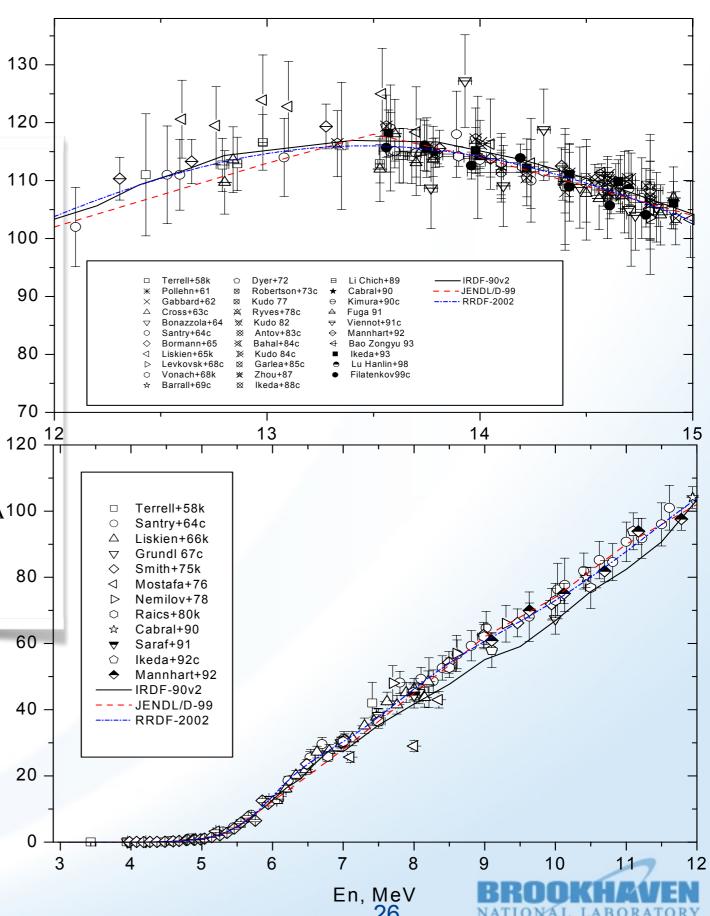


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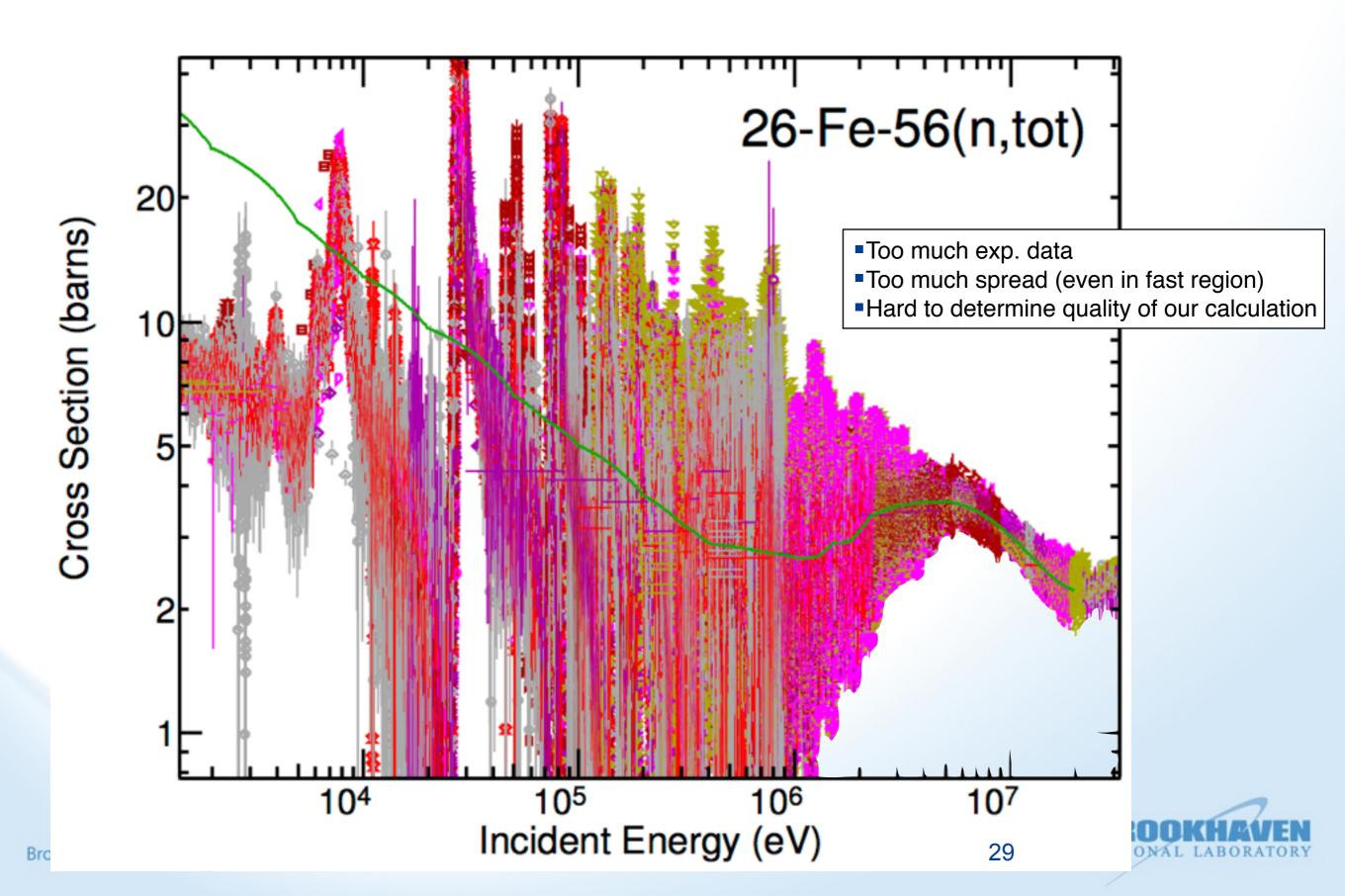
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Summary of EMPIRE input

- CC for incident/outgoing channels + DWBA
- Soukhovitskii and Capote dispersive OMP
- Microscopic HFB level densities
- Width fluctuation correction (HRTW) up to 8 MeV
- Default gamma-ray strength function (Plujko MLO1)
- Multistep Direct/Compound above 3 MeV
- Compressional form factor for the ℓ = 0 transfer
- Exciton model (PCROSS) free path for PE set to 2.5
- Energy-dependent reduction of (n,tot) up to 3 MeV
- Fitted HFB pairing-like and pseudo-a parameters for ⁵⁶Mn
- Minor fit of ⁵⁶Fe level density

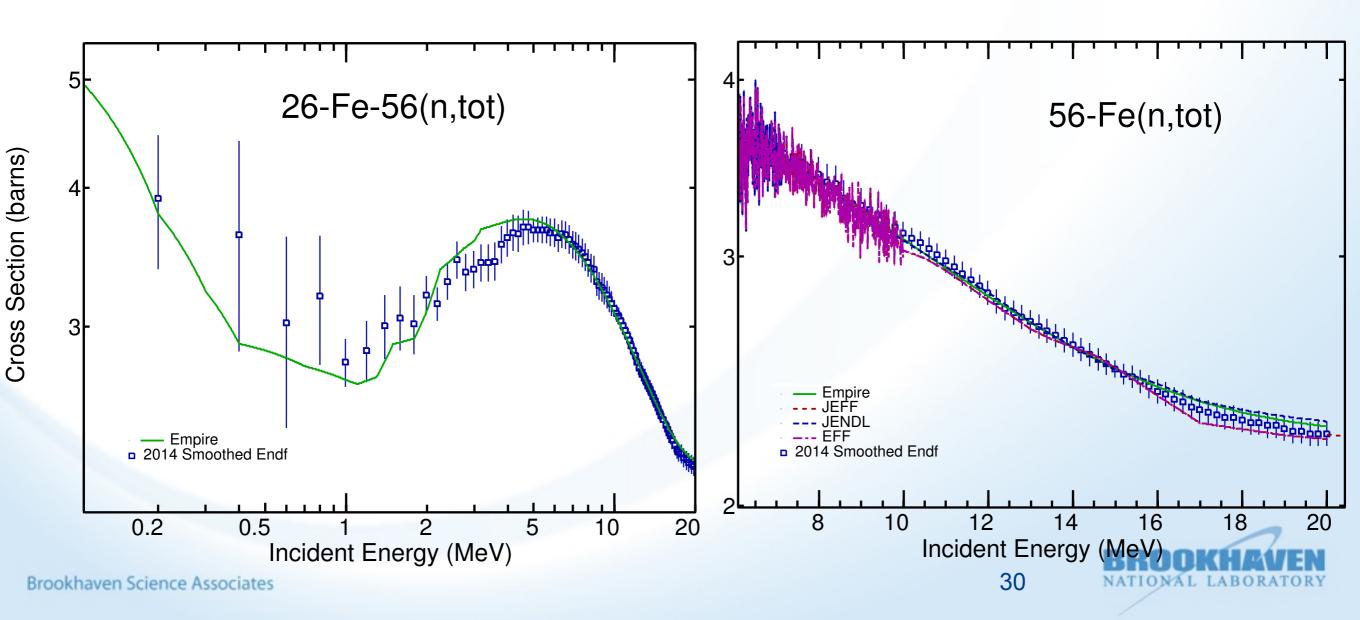


Total cross section

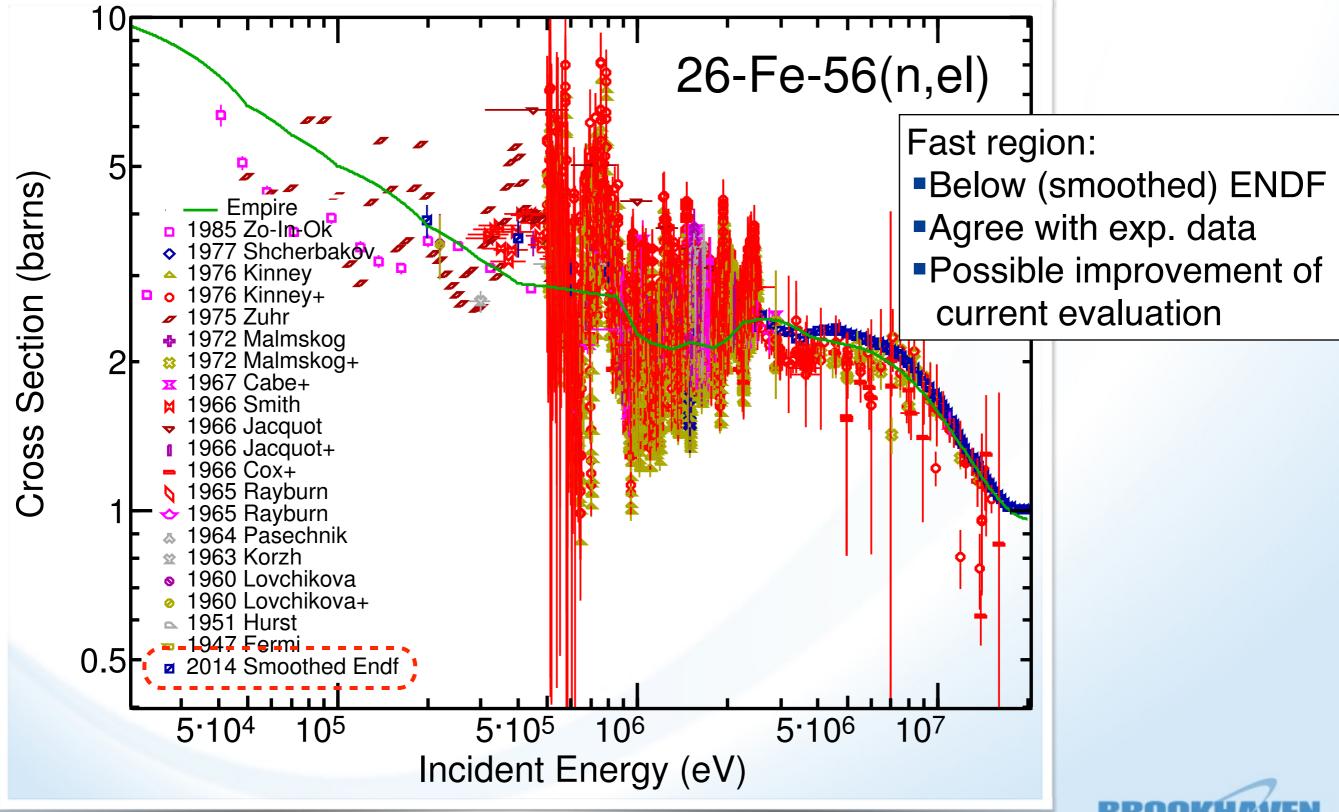


Total cross section

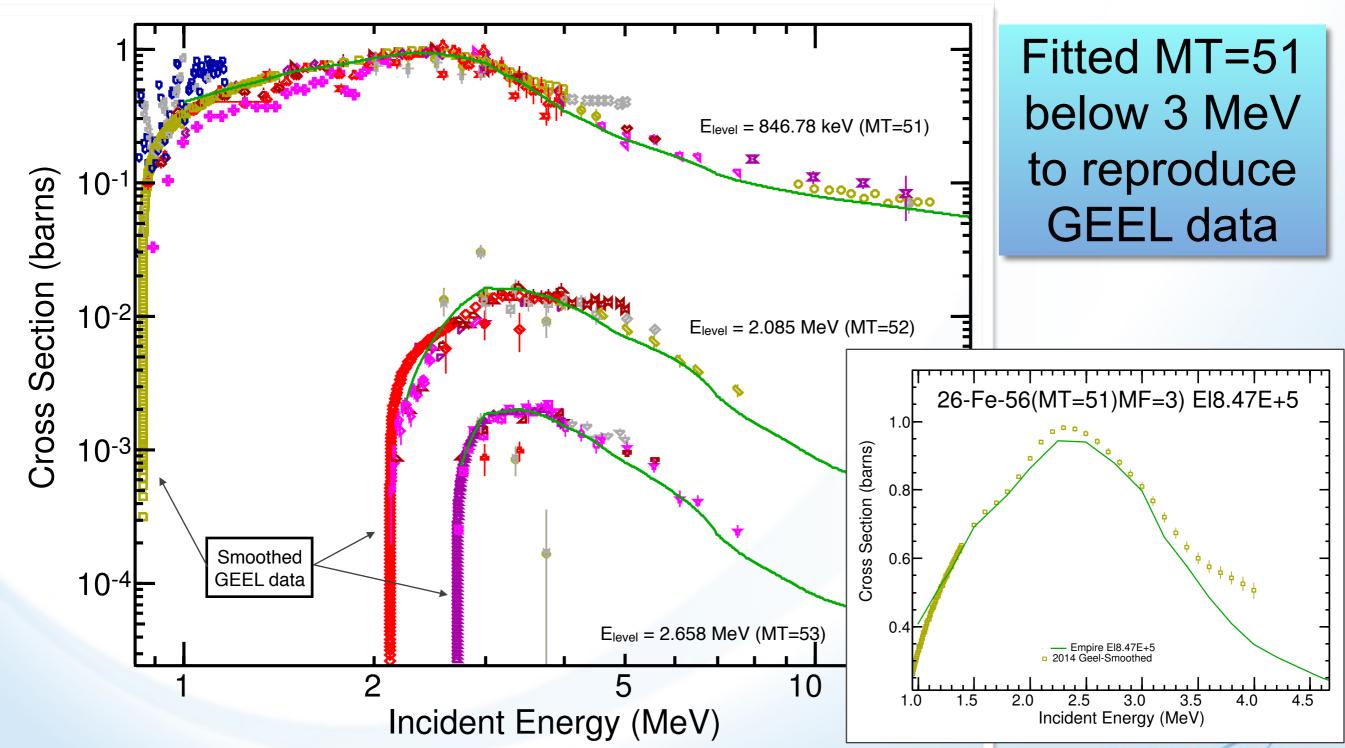
- Smoothed ENDF/B VII.1
- Fitted total below 3 MeV
- For higher energy, we are in good agreement with previous evaluations



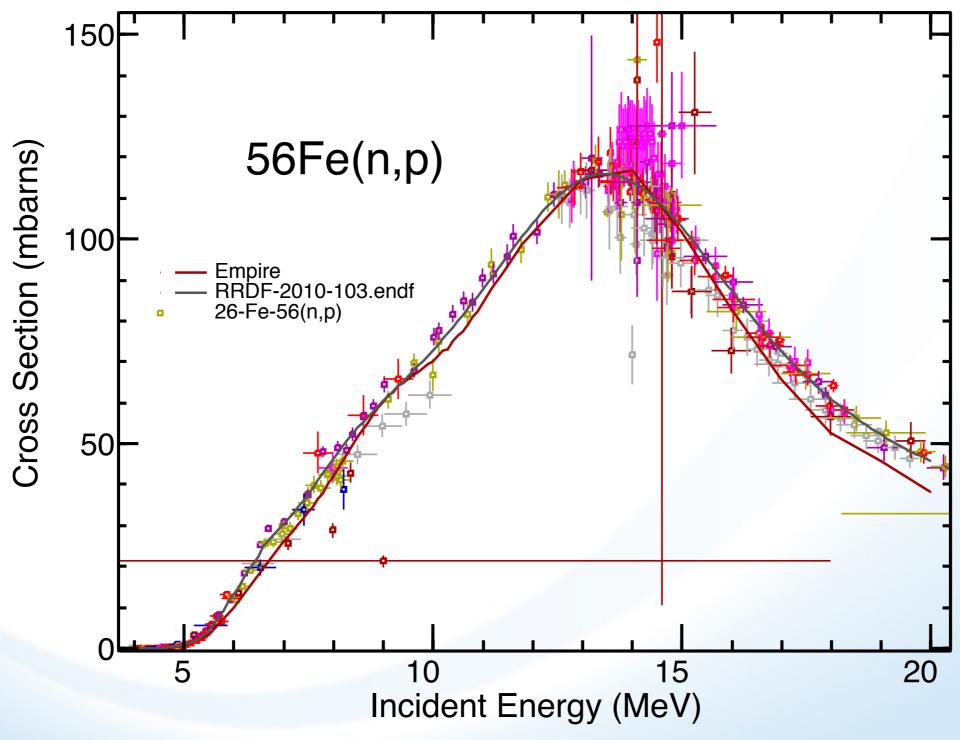
Elastic cross section



Inelastic cross sections

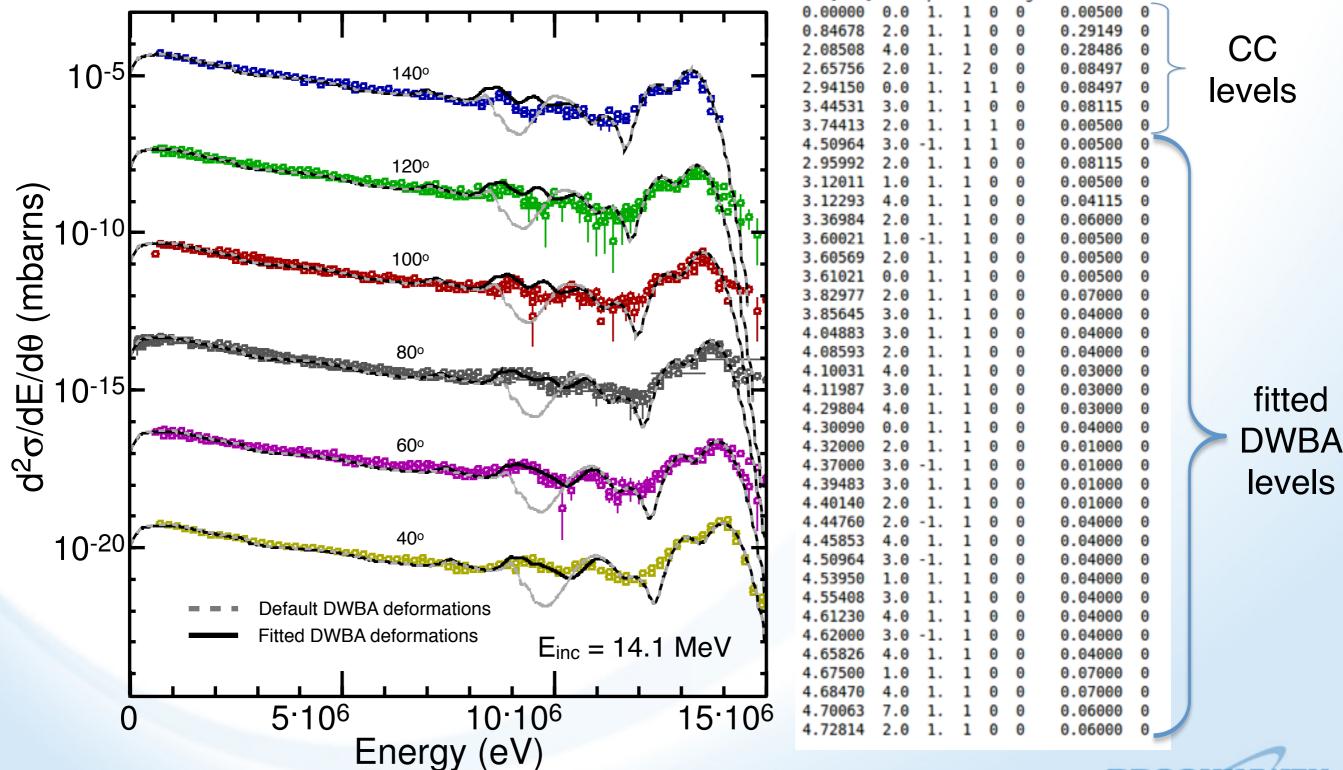


⁵⁶Fe(n,p) comparison with IRDFF (RRDF-2010) - still some work to do...

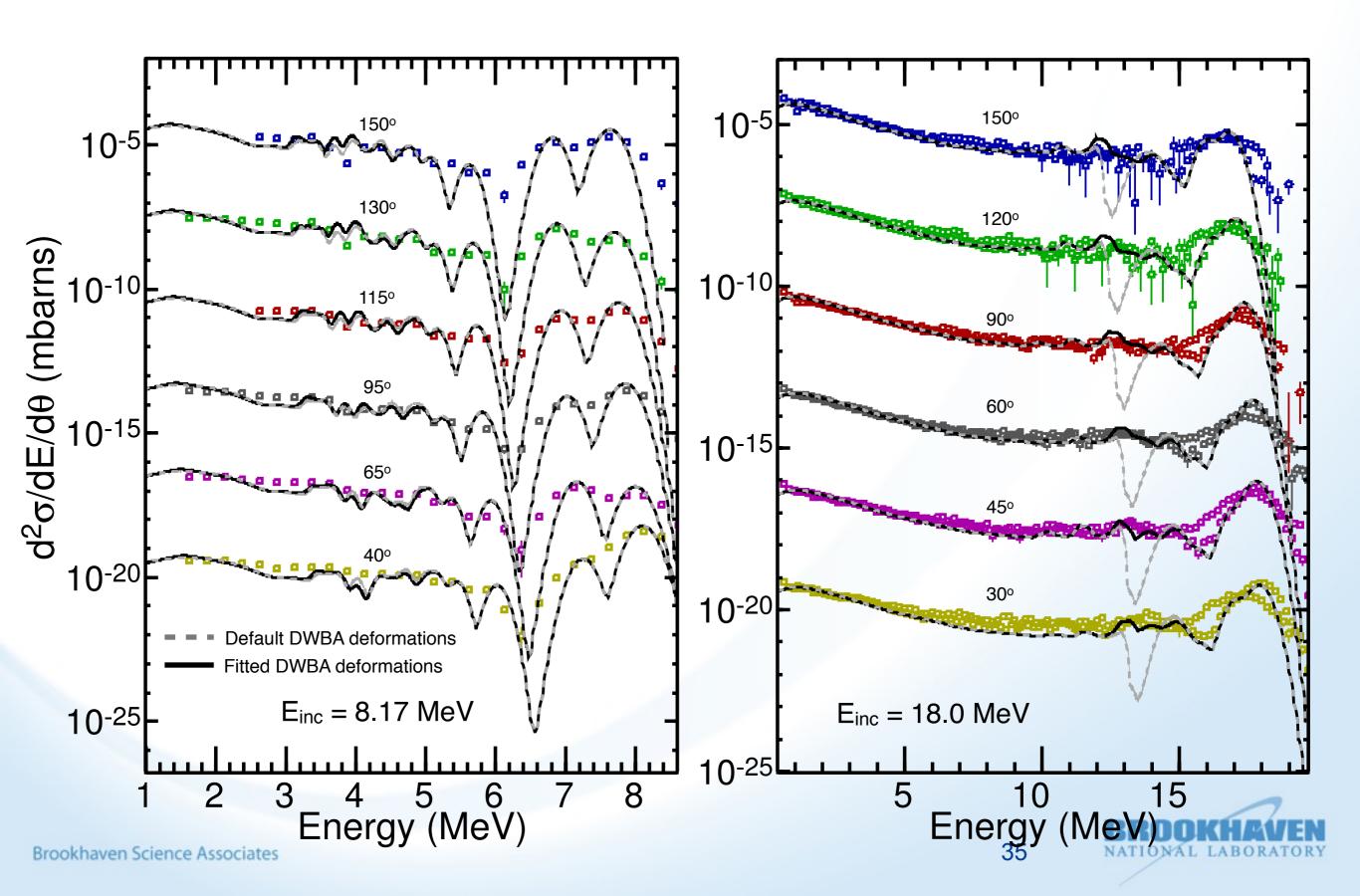




Double-differential cross sections



Double-differential cross sections

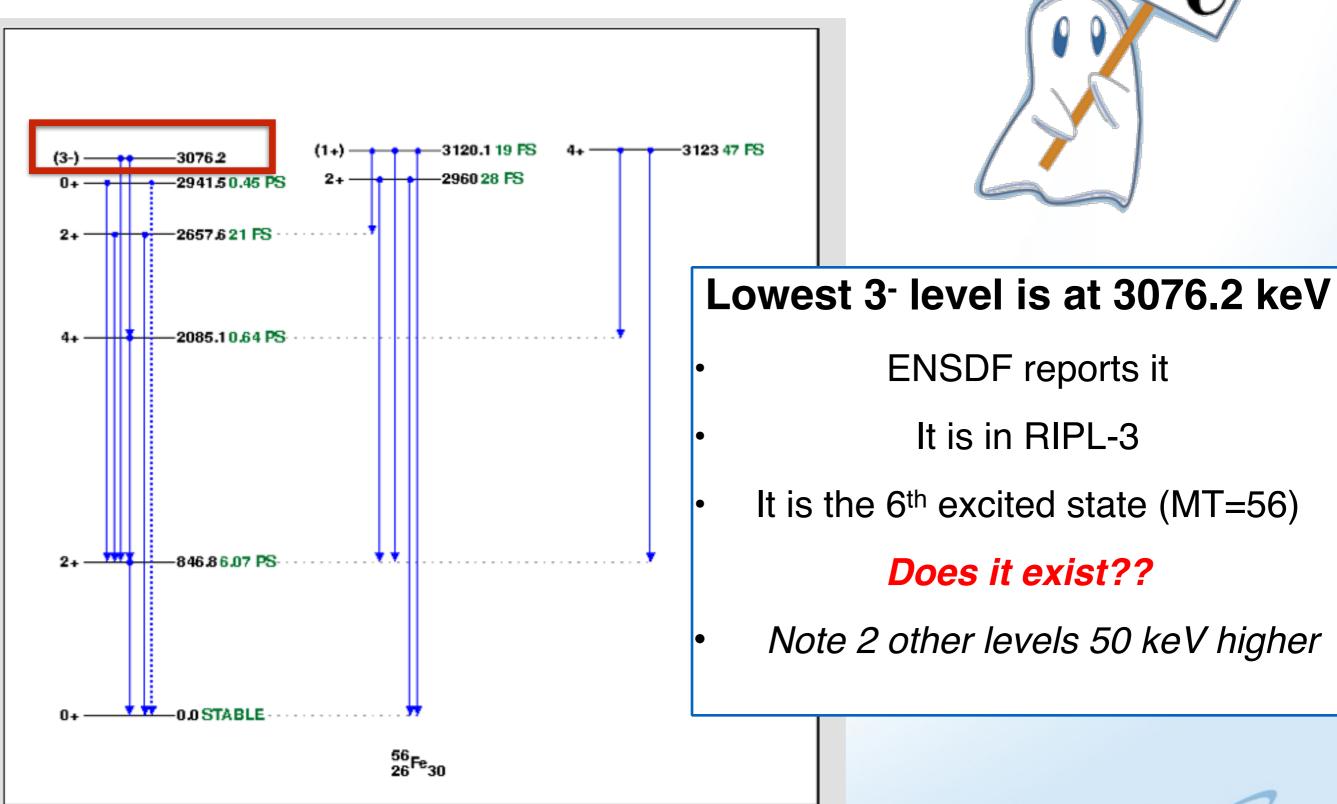


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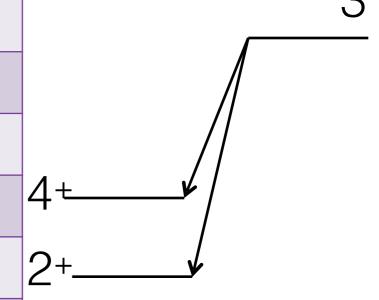
The spooky mystery level



Origin of level in ENSDF

Appears to be observed in 7 different reactions

57	3090	L=1	
56	3070	L=(3)	
54	3100 (50)	L=4	
56	3100	L=3	
60	3070 (30)		
Ni(π	Not observed		
55	3076.2 (4)		



	$E_{\mathbf{p}}$:	1435	1441 b)	1446 b)	1452	1455b)	1460
J_{f}^{π}	E_{x}	11593	11599	11603	11609	11613	11618

the very strong primary transition to the 4100 keV level and other two peaks are probably weak. However, the level is evidently excited by secondary transition from the intensely excited 5503 and 5670 keV and from rather weakly excited 6048 keV levels, although all corresponding peaks are strongly contaminated by other transitions. In contradiction with Ref. [7] intensity of the 2229 keV transition established in the present work is low and is nearly exhausted by decay of other levels. Rather strong 991 keV nearly pure γ -peak has been observed at all resonances with similar intensity. This might indicate that this peak is connected with the low-lying level and is a good candidate for the decay of the 3077 keV level to the 2085 keV state.

Only level seen in just one resonance

Fotiades et al., thoroughly refute it

PHYSICAL REVIEW C 81, 037304 (2010)

First 3⁻ excited state of ⁵⁶Fe

N. Fotiades,* R. O. Nelson, and M. Devlin Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA (Received 4 February 2010; published 31 March 2010)

There is no reliable evidence for the existence of the 3.076 MeV (3⁻) level adopted in the ENSDF ev for 56 Fe although it has been reported in a few experiments. Previous reports of the observation of this leve to be based on an incorrect assignment in early (e, e') work. Recent neutron inelastic scattering measurer Demidov *et al.* [Phys. At. Nucl. **67**, 1884, (2004)] show that the assigned γ -ray decay of this state does reported in the ENSDF evidence of the control of the existence of the 3.076 MeV (3⁻) level adopted in the ENSDF evidence of the control of the existence of the 3.076 MeV (3⁻) level adopted in the ENSDF evidence of the control of the control of the existence of the observation of this level to be based on an incorrect assignment in early (e, e') work. Recent neutron inelastic scattering measurer of the control of the existence of the control of the control of the control of the existence of the control o

at a level consistent with known properties of inelastic scattering. In the present work the 56 Fe(n, $n'\gamma$) reaction was used to populate excited states in 56 Fe. Neutrons in the energy range from 1 to 250 MeV were provided by the pulsed neutron source of the Los Alamos Neutron Science Center's WNR facility. Deexciting γ rays were detected with the GEANIE spectrometer, a Compton suppressed array of 26 Ge detectors. The γ - γ data obtained with GEANIE were used to establish coincidence relations between transitions. All previously reported levels up to $E_x = 3.6$ MeV excitation energy were observed except for the 3.076 MeV (3 $^-$) level. The 991- and 2229-keV transitions, previously reported to deexcite this level, were not observed in the γ - γ coincidence data obtained in the present experiment. The present work supports the assignment of the 4509.6 keV level as the first 3 $^-$ excited state in 56 Fe by observation of two previously known transitions deexciting this state.

(n,n'γ) experiment

Non-observation of 2 depopulating transitions

The true ghost-buster



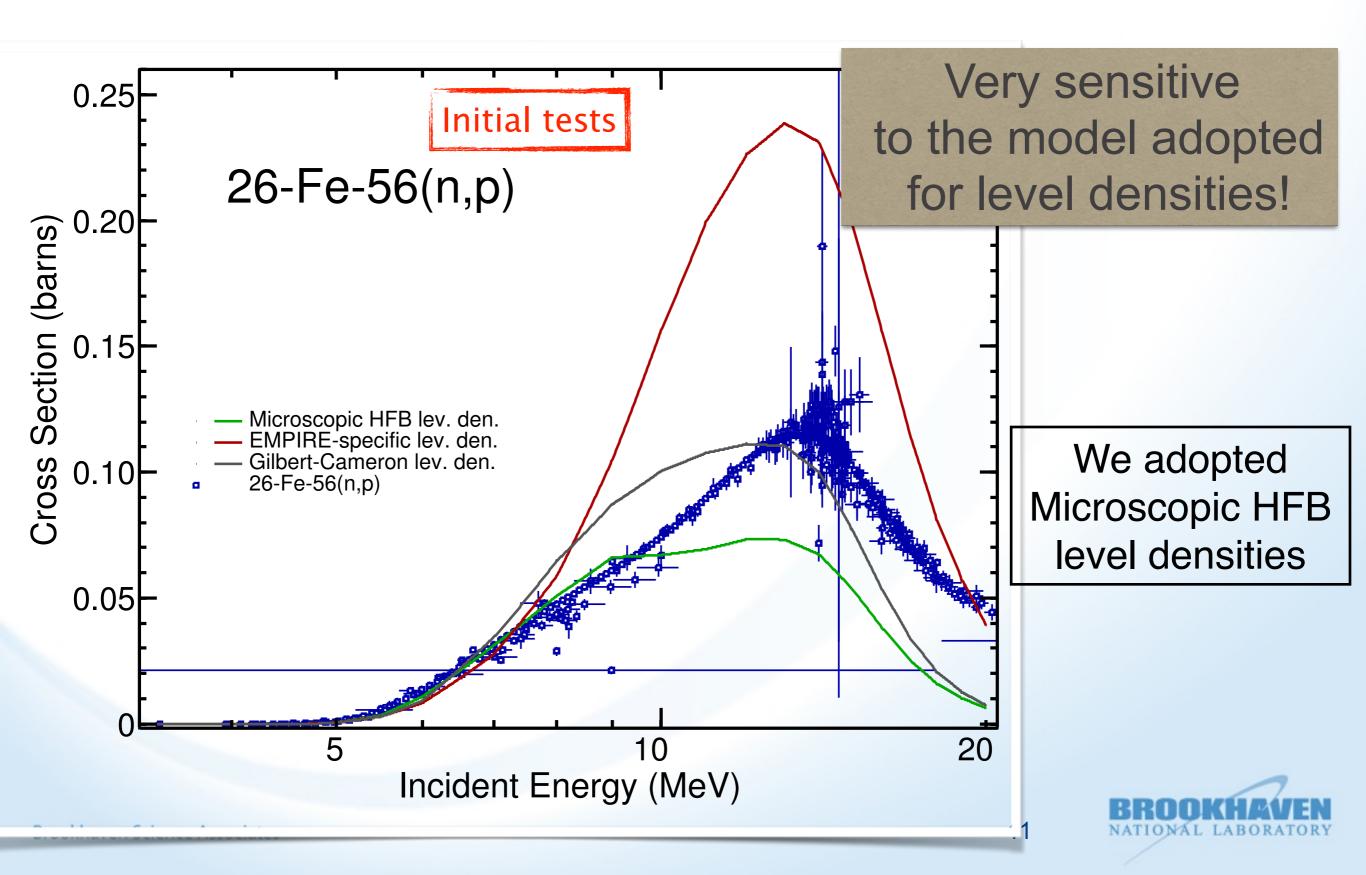
- Repeat (p, γ) experiment with γ- γ coincidences
- Easy experiment for facility with small tandem

Along the way we have:

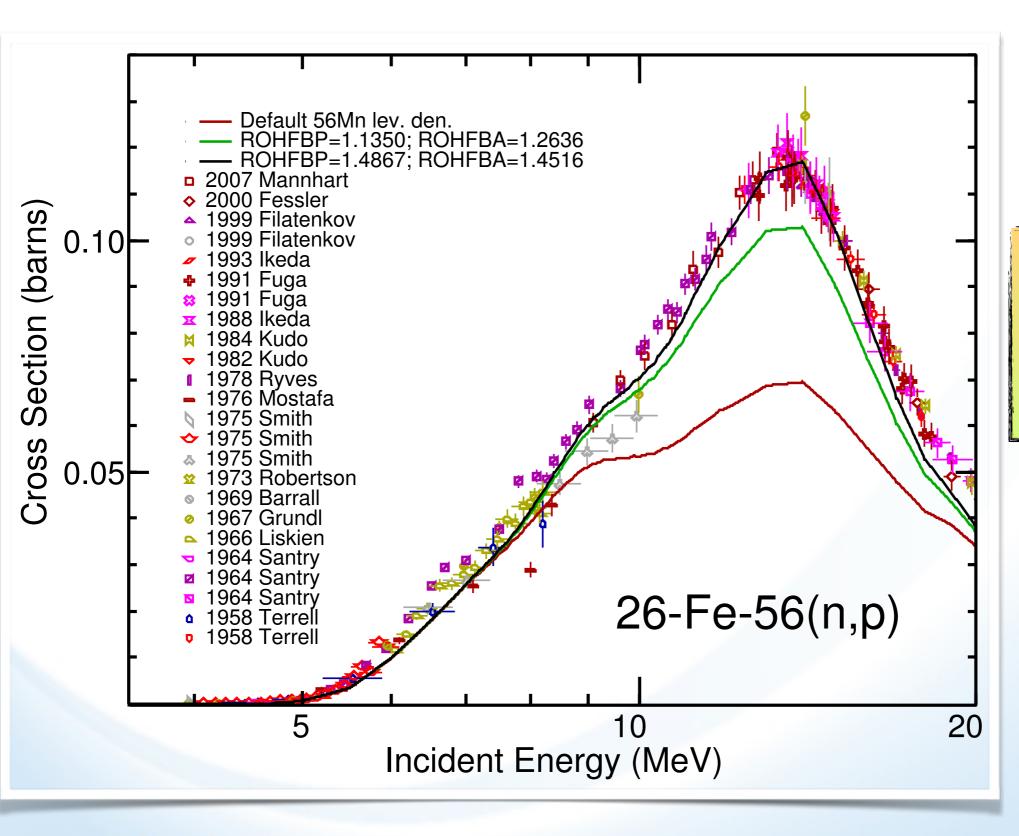
- solved mystery in the ENSDF/RIPL 56Fe level scheme
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⁵⁶Fe(n,p) - level-density models



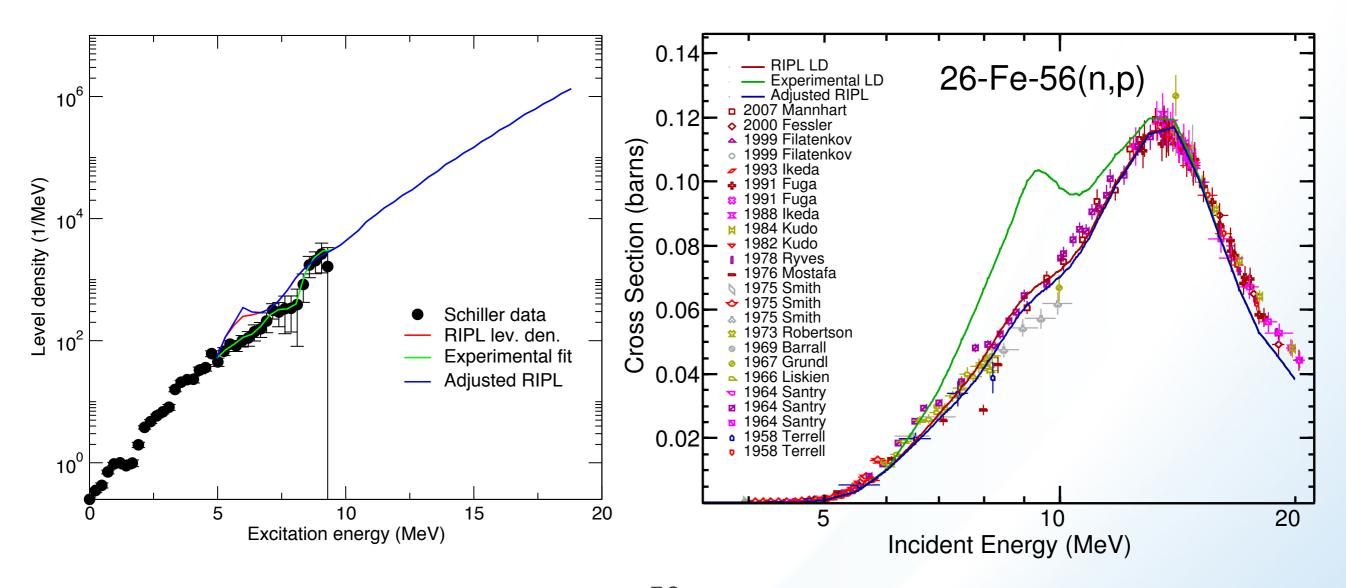
⁵⁶Fe(n,p) sensitivity to ⁵⁶Mn lev. den.



⁵⁶Fe(n,p) is very sensitive to ⁵⁶Mn level-density parameters



⁵⁶Fe(n,p) sensitivity to ⁵⁶Fe lev. den.



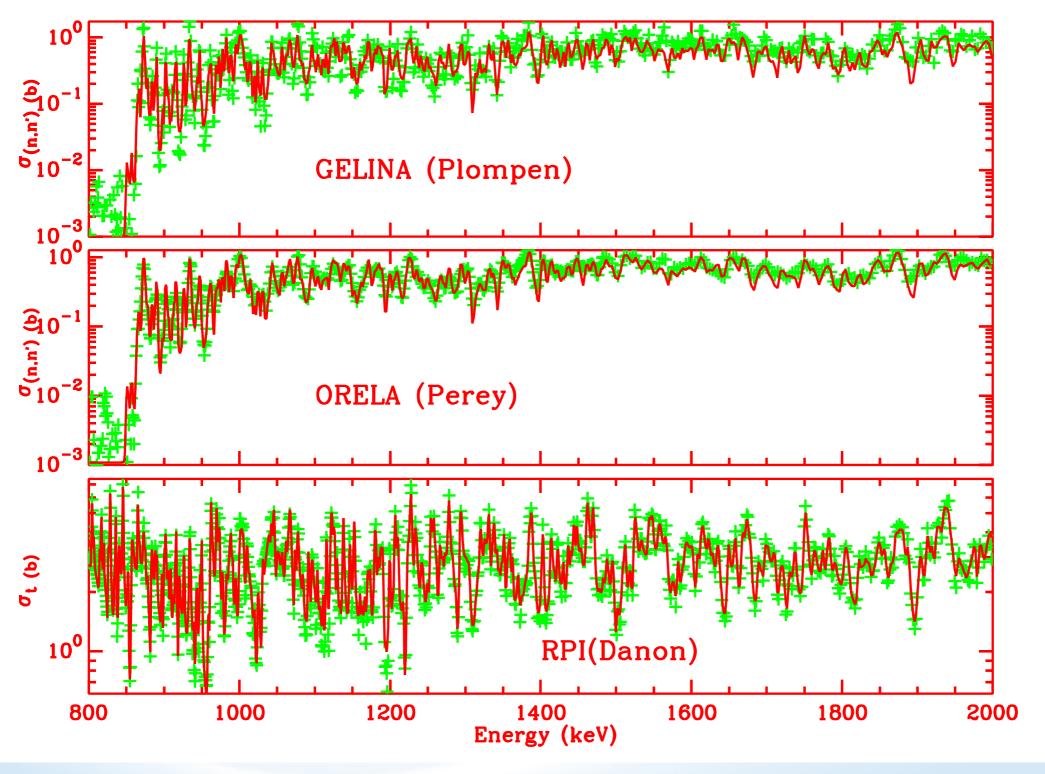
- Also incredibly sensitive to ⁵⁶Fe level density.
- Center of experimental LD leads to poor (n,p).
- Tweaks on LD can significantly change (n,p).



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Must merge onto L. Leal's 56Fe RRR



It is beautiful,

- LRF=7,
- extends to2 MeV
- Includes
 (n,tot),
 (n,el),
 (n,γ),
 (n,n₁')
- If not all RRR exp. data, at least most of it
- Fitted angular dists. too



To match onto Leal's RRR, must smooth cross sections

- OMP & Hauser-Feshbach theory only tell us about average cross sections
- Preferred averaging is with Lorenzian:

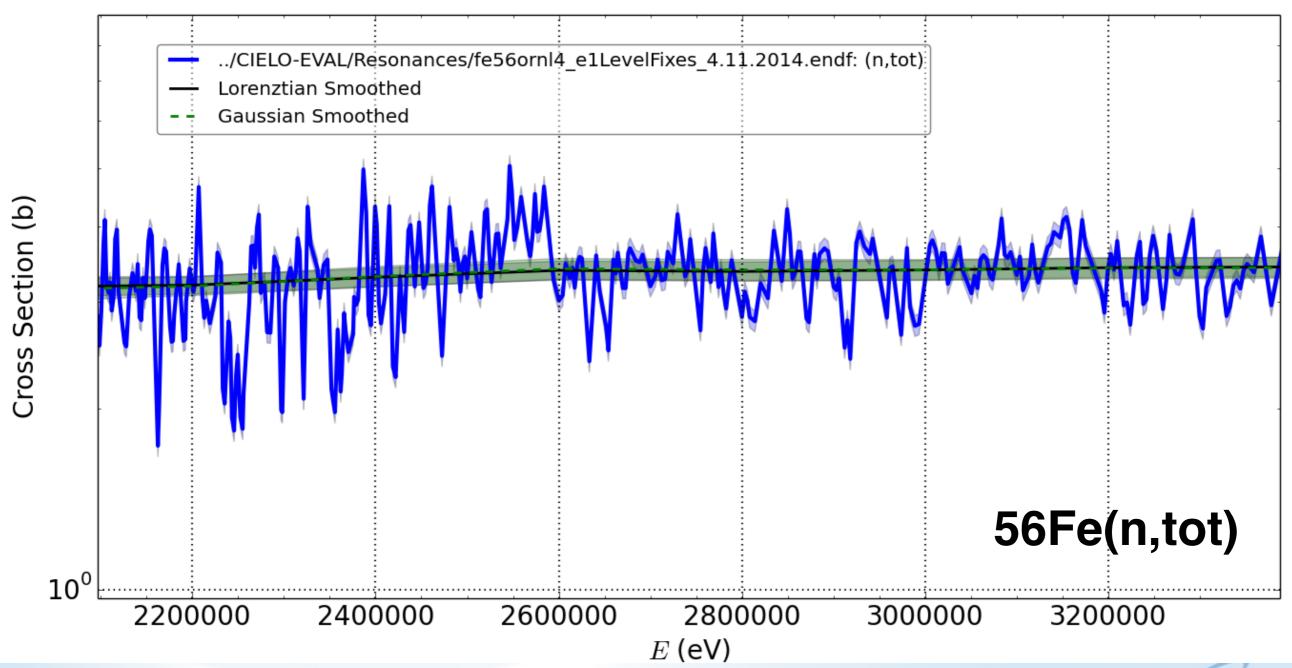
$$L(E, E') = \frac{1}{\pi} \frac{I}{(E' - E)^2 + I^2}$$

so that averaged have nice mathematical properties:

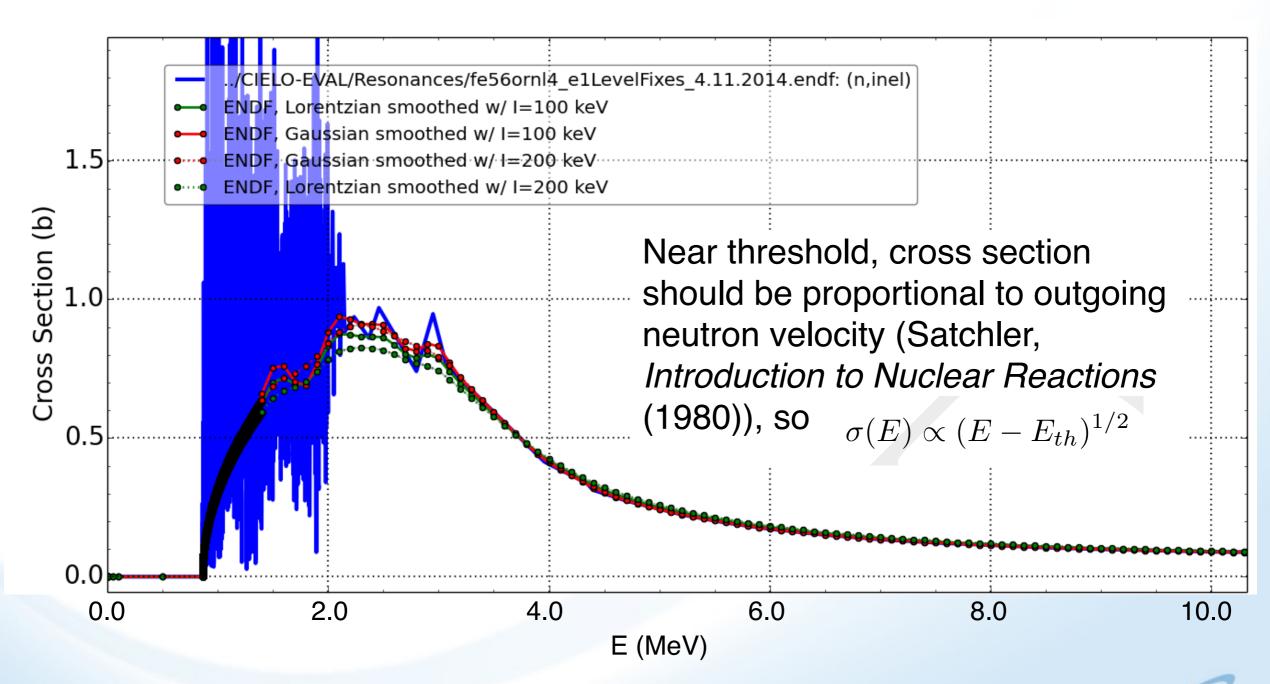
$$\langle f(E) \rangle = \int_{-\infty}^{\infty} dE' L(E, E') f(E')$$

$$= f(E + iI)$$

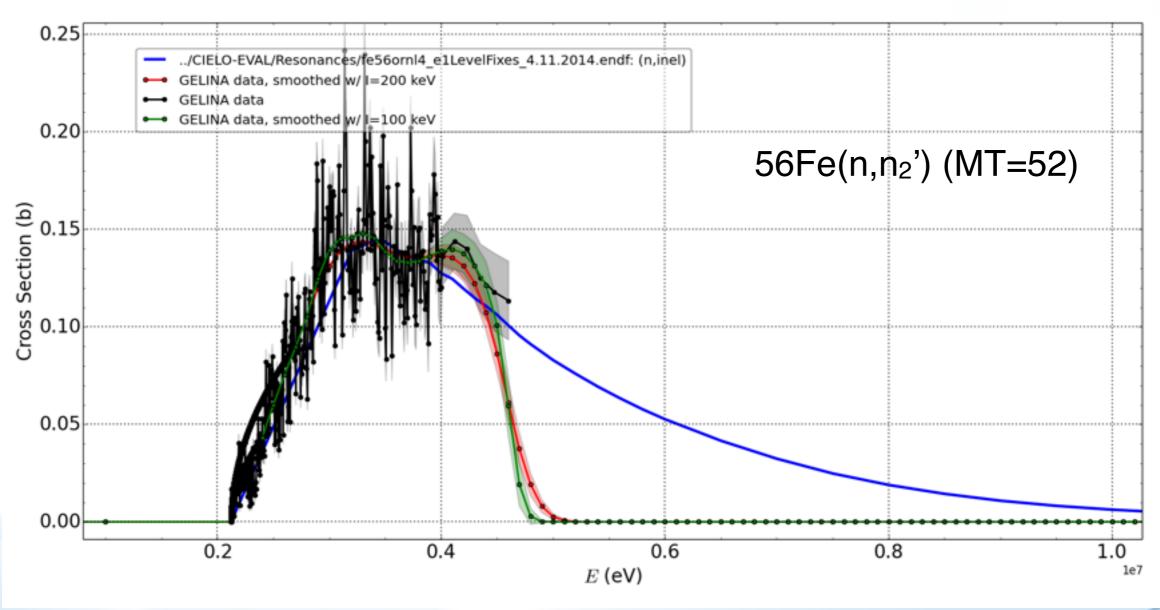
Turns out smoothed cross section rather insensitive to smoothing profile except near discontinuities



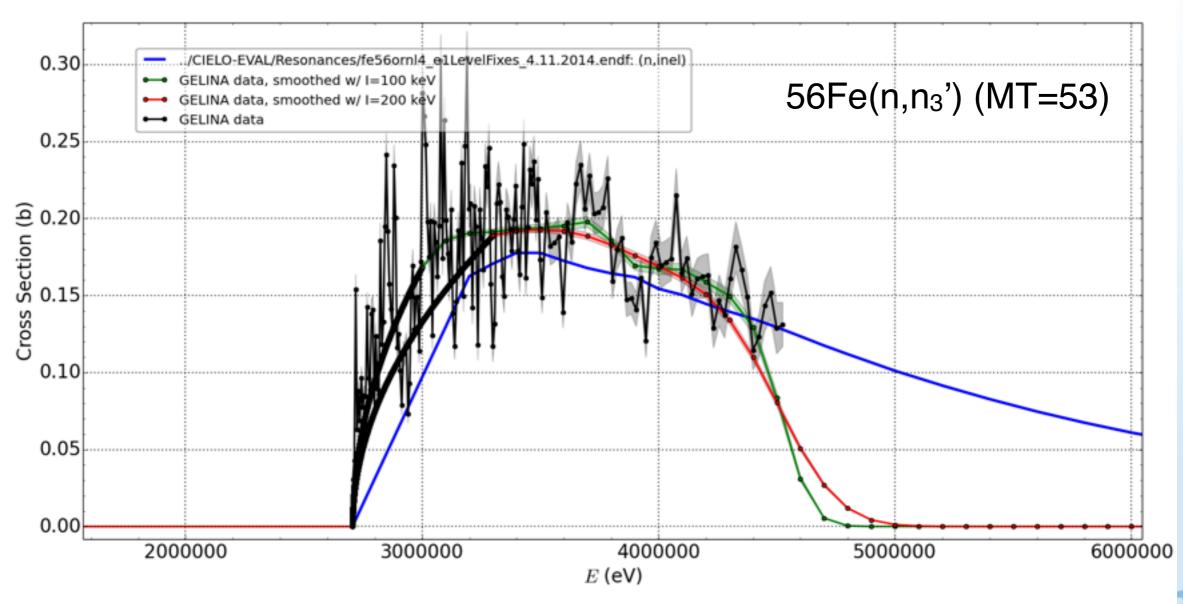
Leal's RRR included MT=51 (n,n₁'); we have to deal with threshold discontinuity



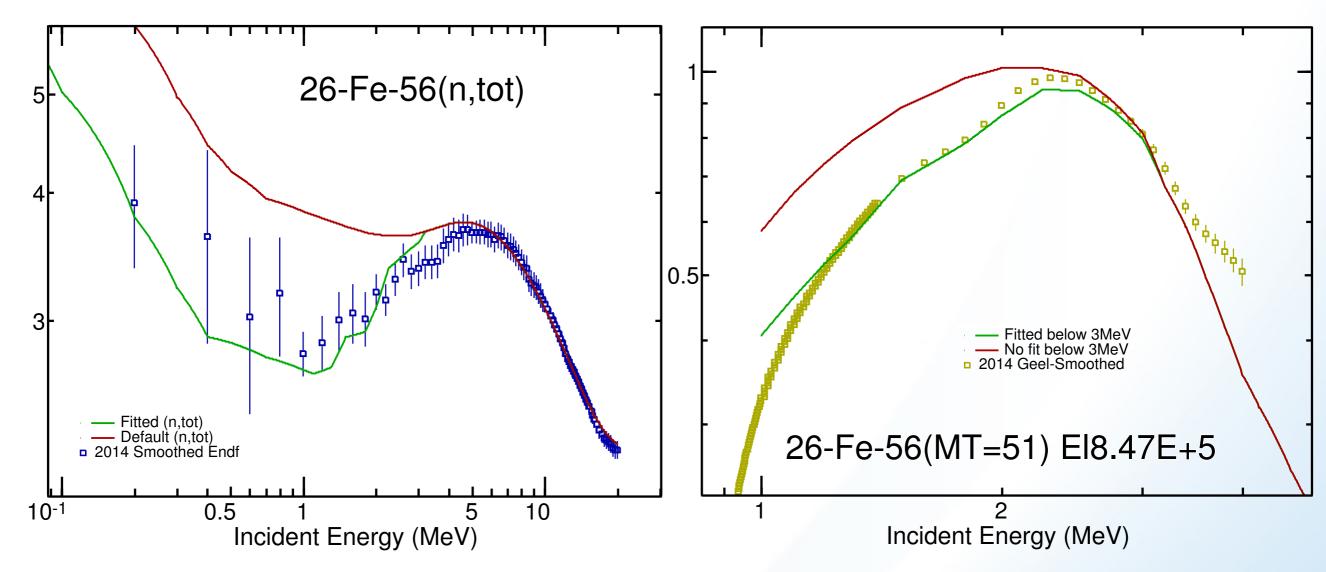
We can use the same procedure on the Geel data to smooth out the experimentally resolved fluctuations in the other inelastic levels



We can use the same procedure on the Geel data to smooth out the experimentally resolved fluctuations in the other inelastic levels



Fit of (n,tot) below 3 MeV



- We simulate Kawano's I-dependent OMP with non-led
 dependent factor
- This way we preserve CN to Shape Elastic ratio and angular distributions

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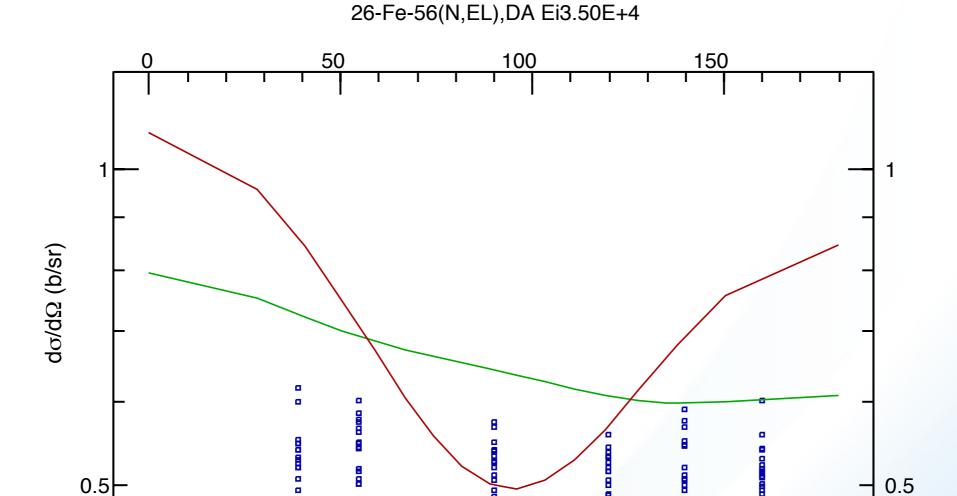
51

Cross Section (barns)

Along the way we have:

- solved mystery in the ENSDF/RIPL 56Fe level scheme
- discovered extraordinary sensitive monitor of level densities
- rediscovered Toshihiko's finding that OM for ⁵⁶Fe fails below 3
 MeV
- got a suspicion that angular distributions might be the key to the good iron evaluation
- realized the importance of having clean, differential data based, evaluation for being able to perform future updates



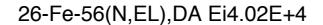


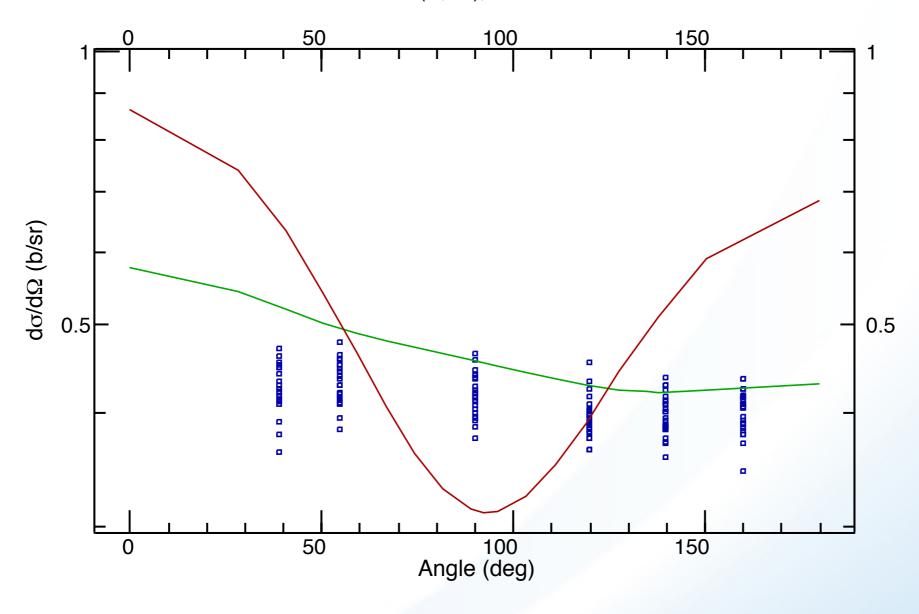
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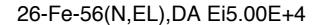
Angle (deg)

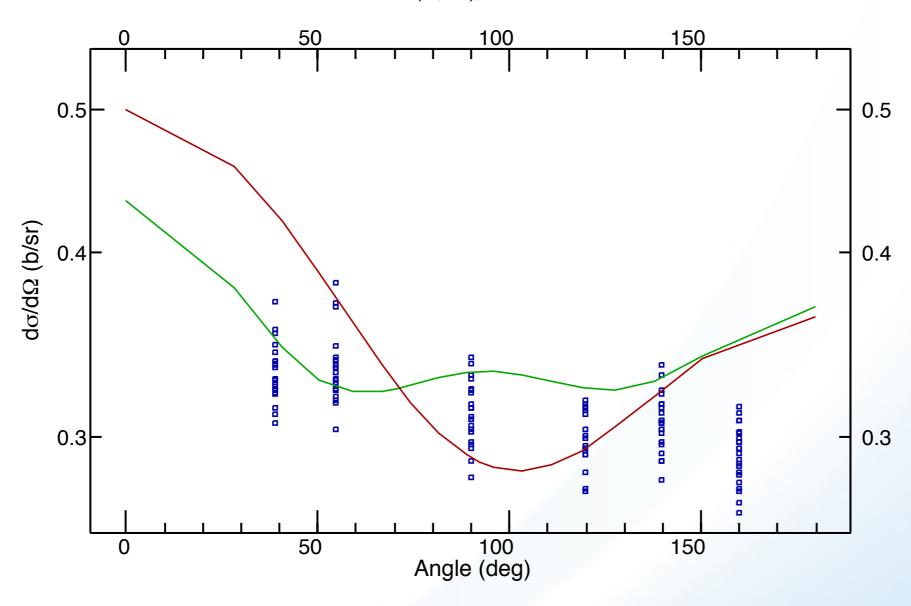
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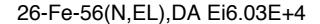
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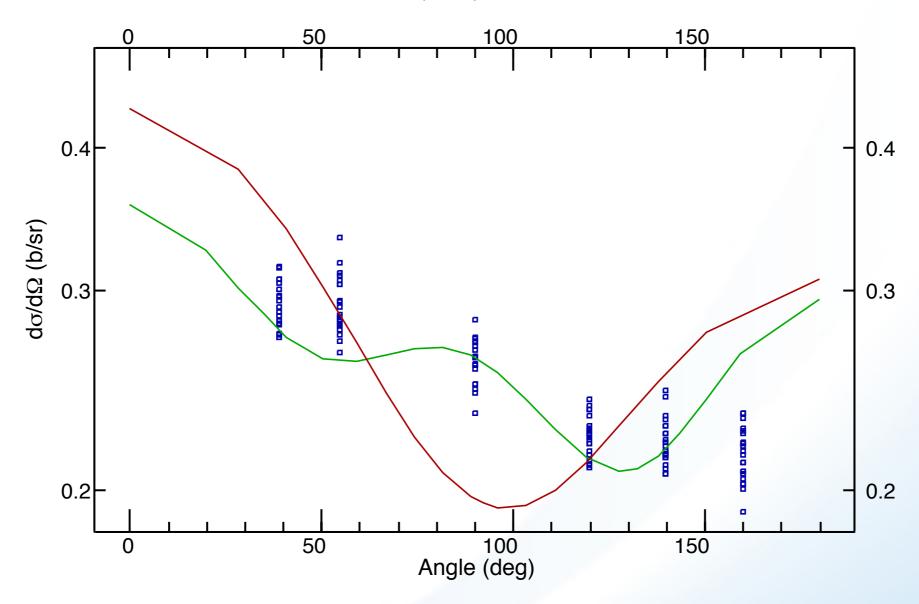


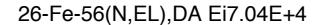


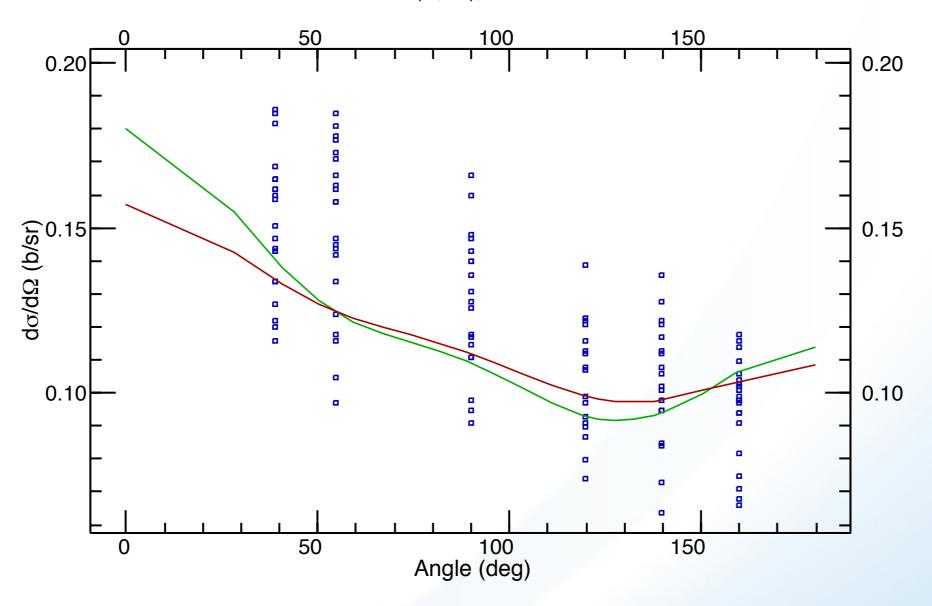


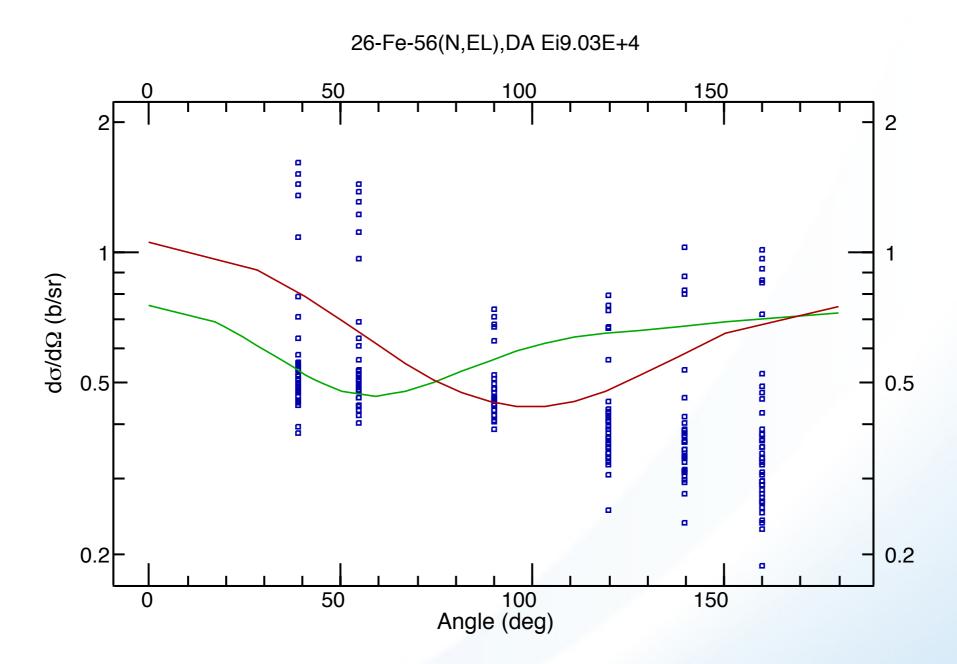


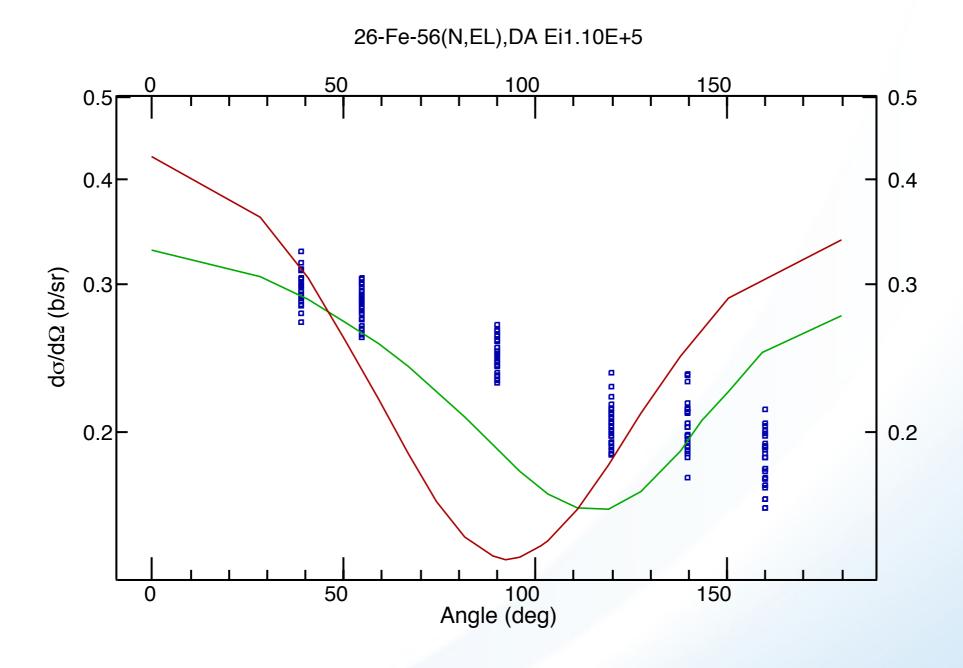


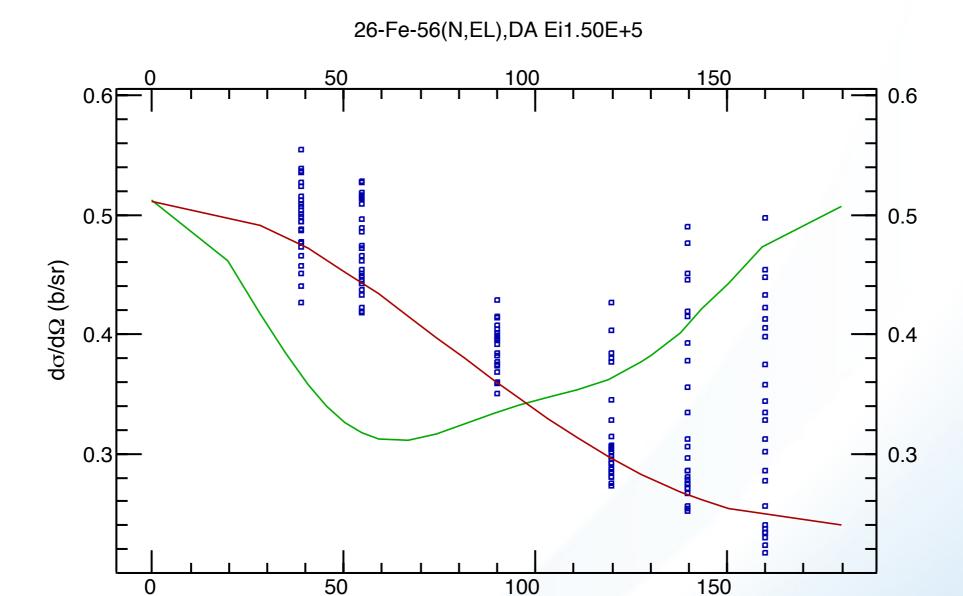




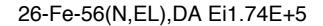


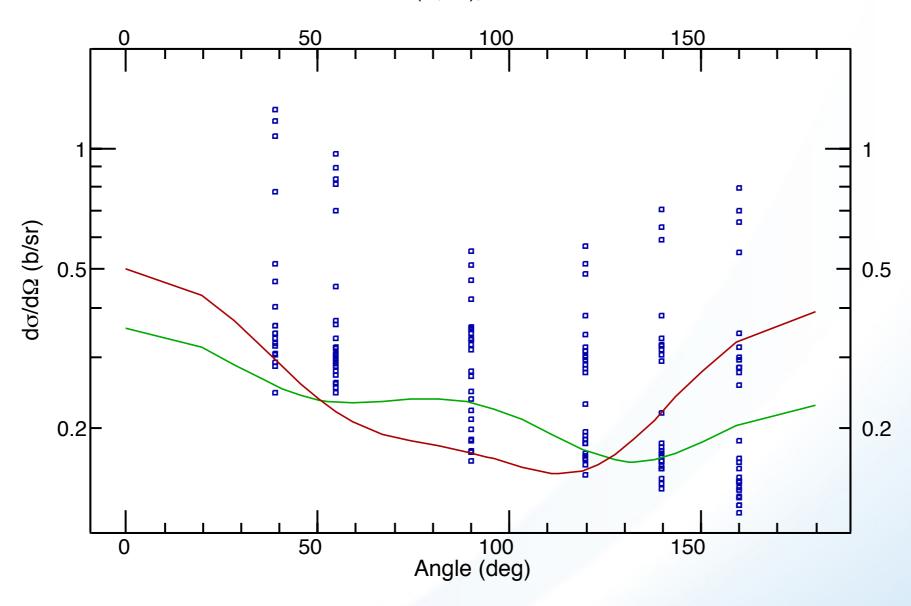


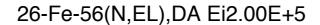


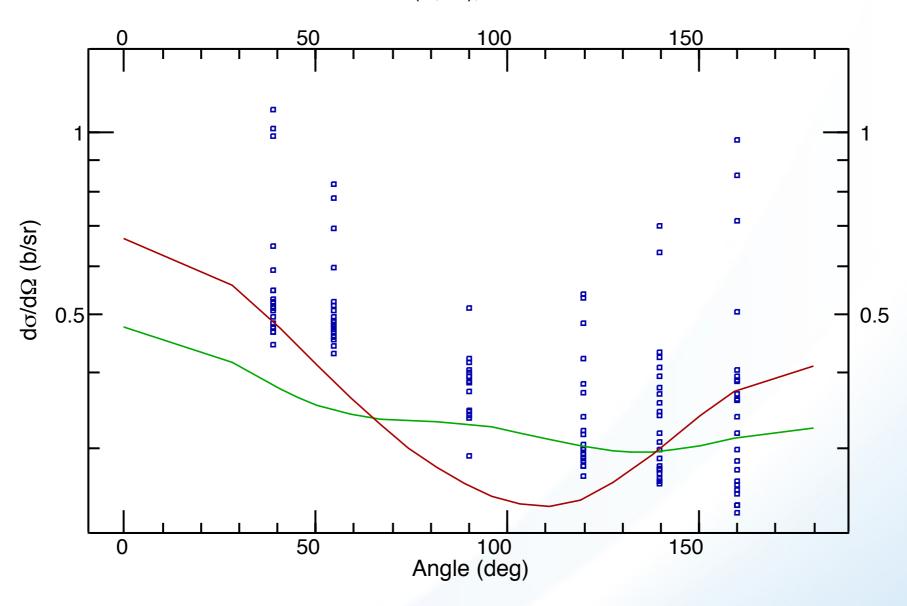


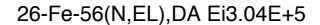
Angle (deg)

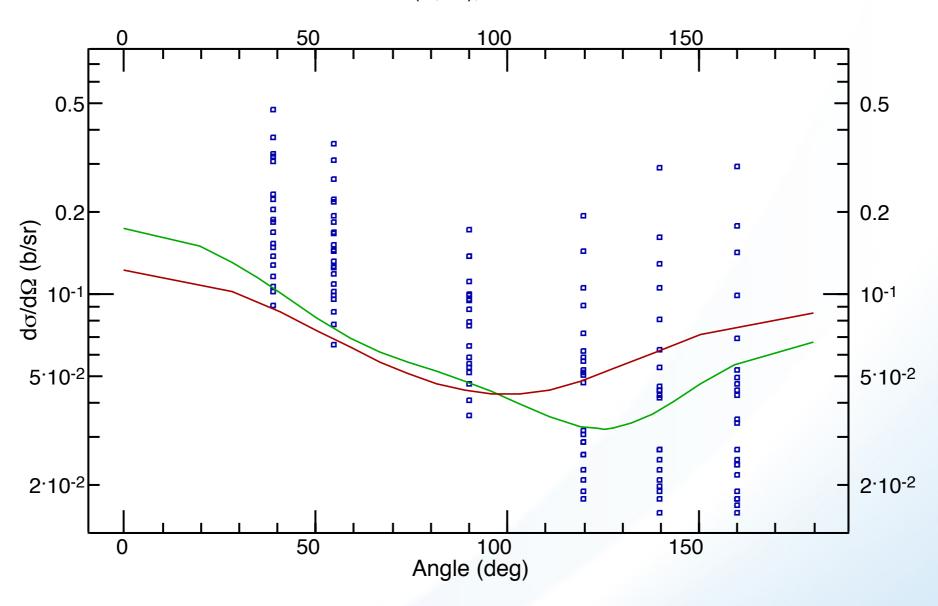


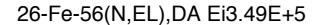


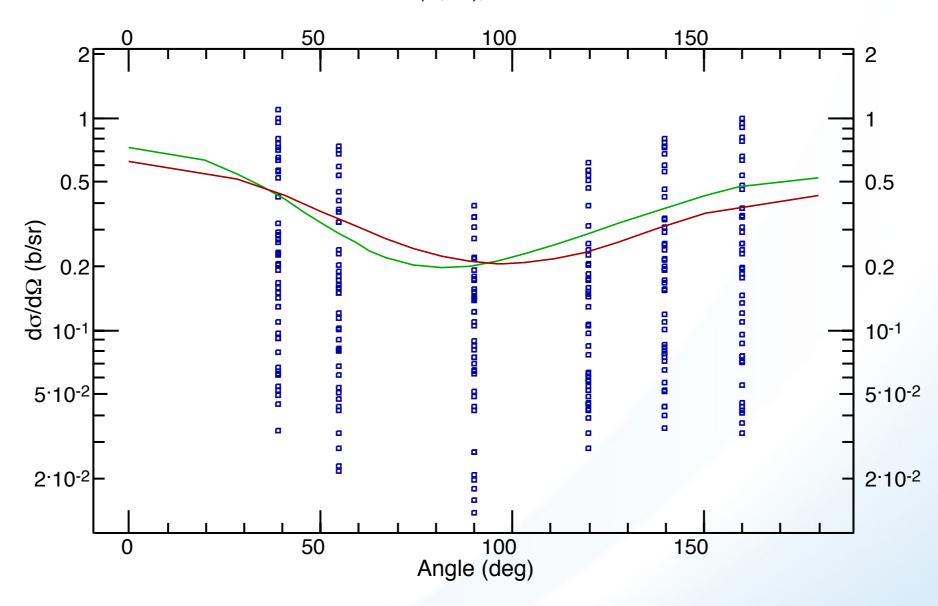


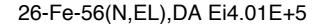


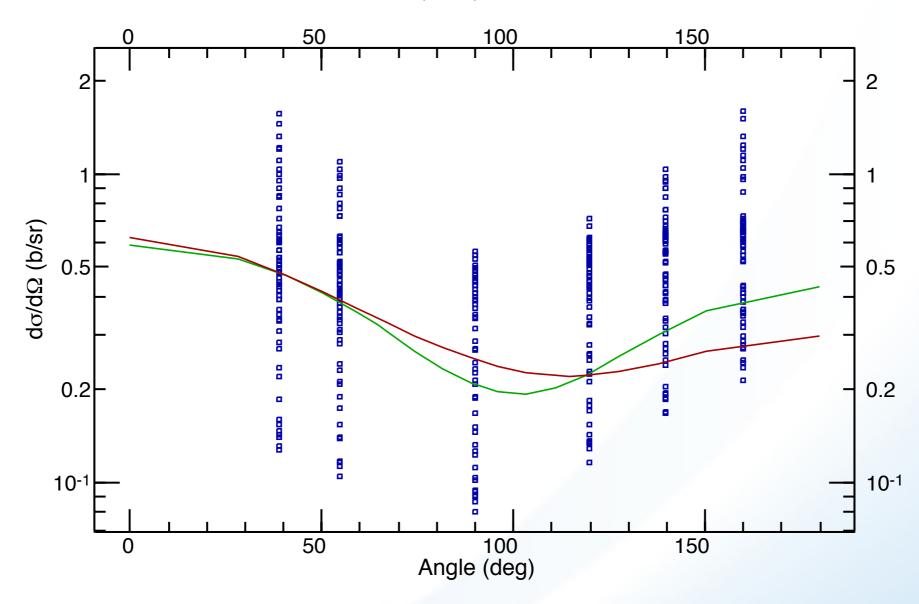


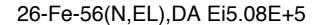


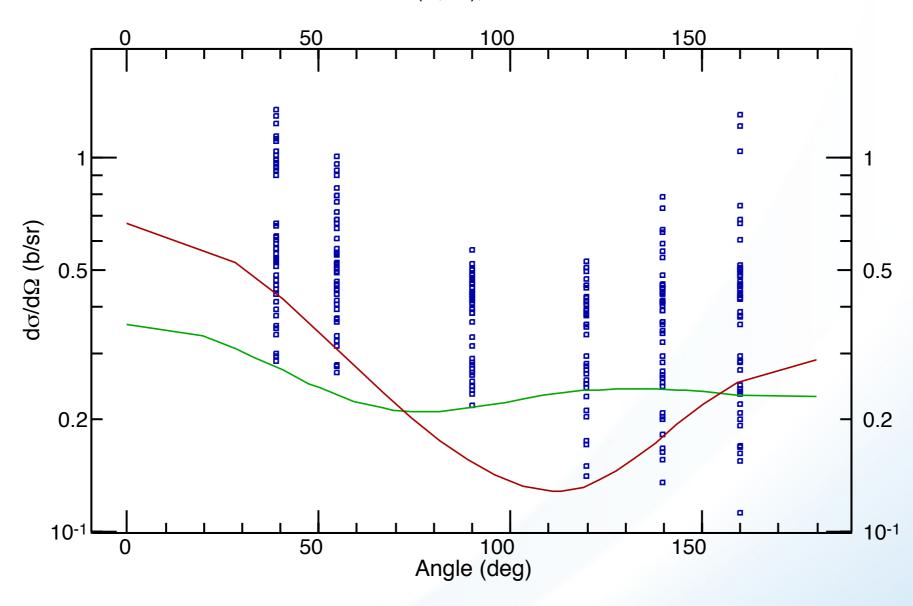


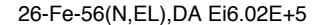


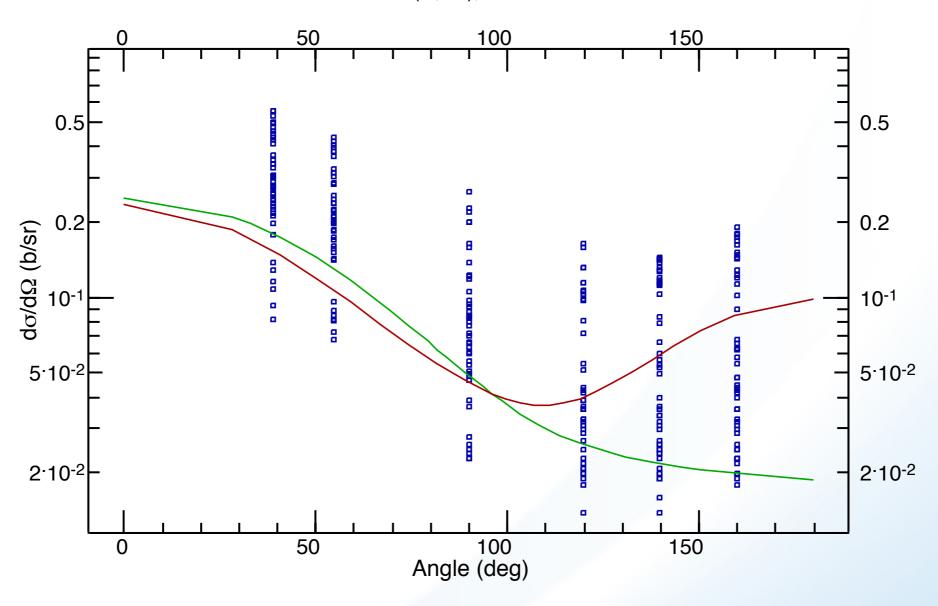


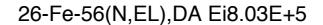


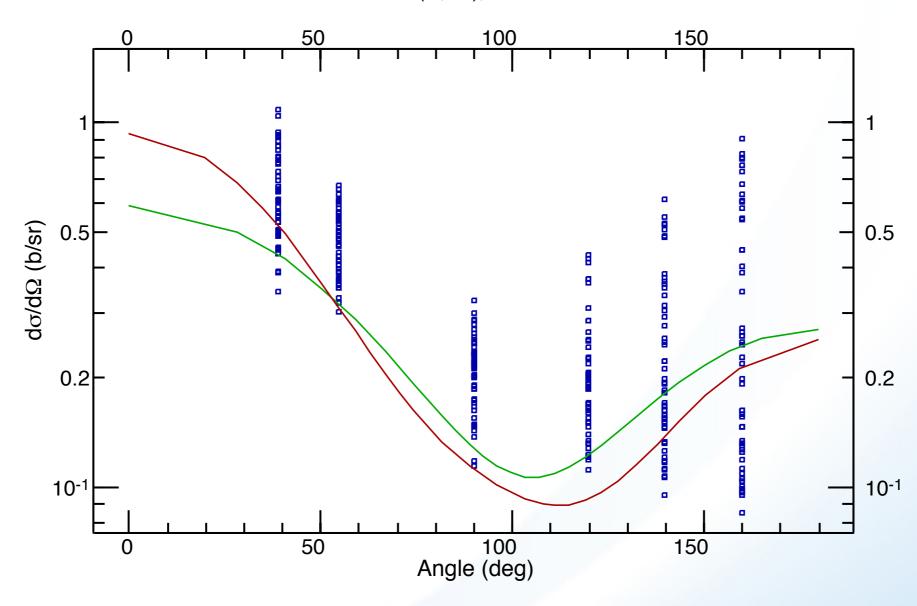


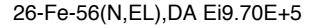


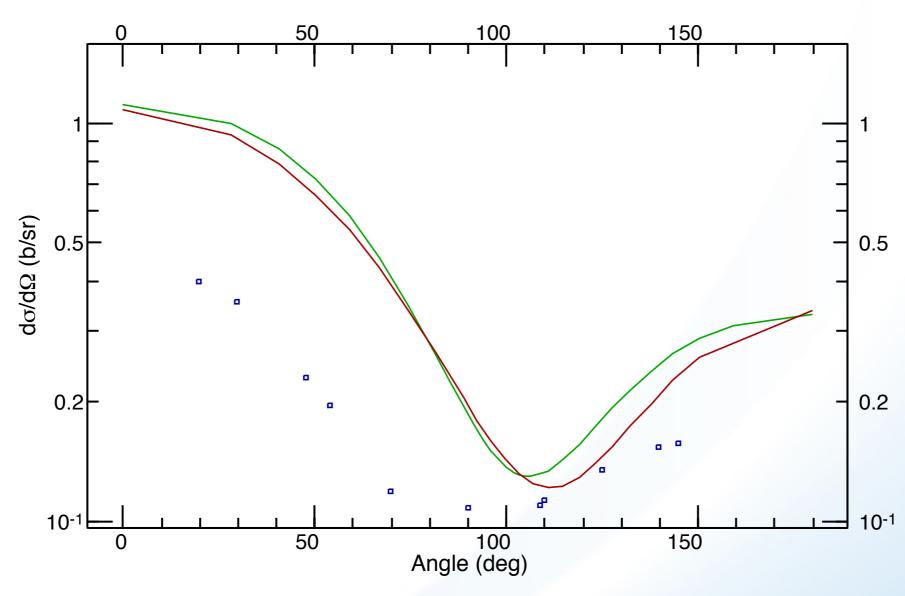


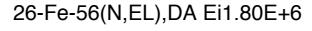


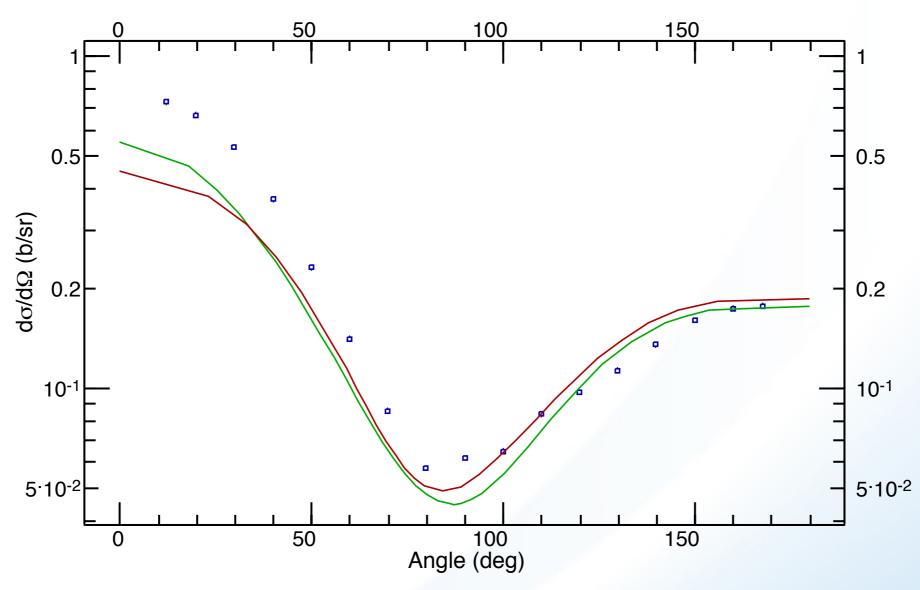


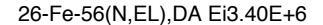


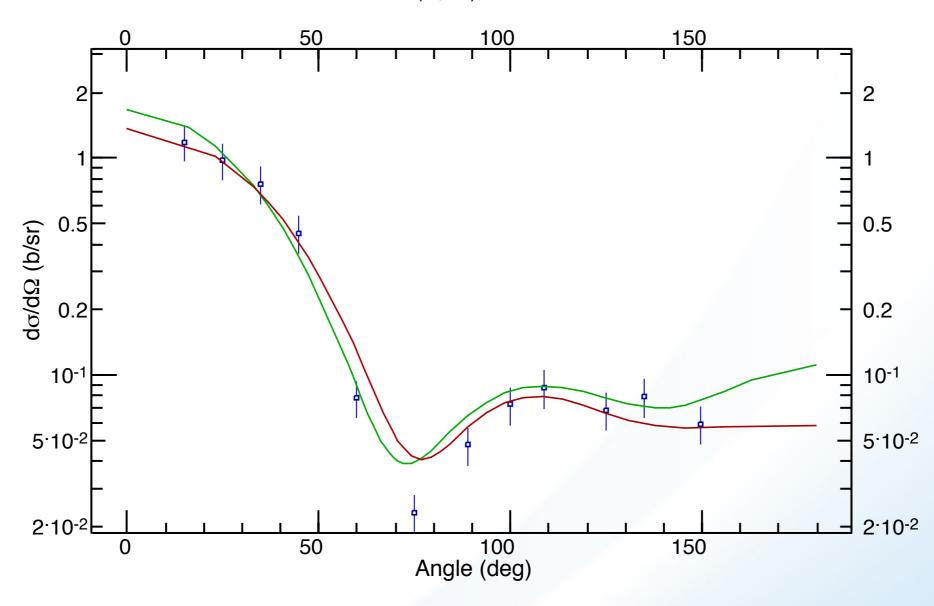






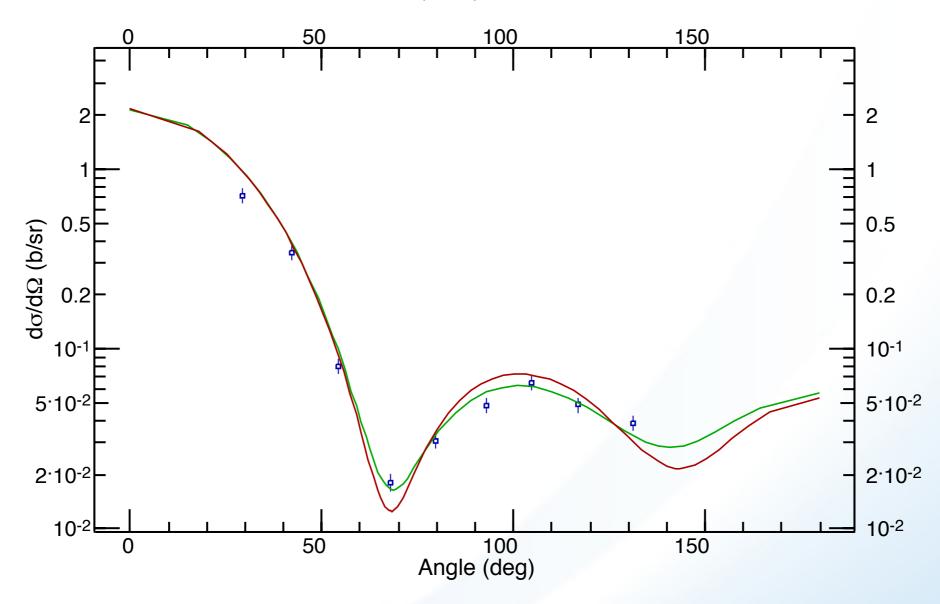




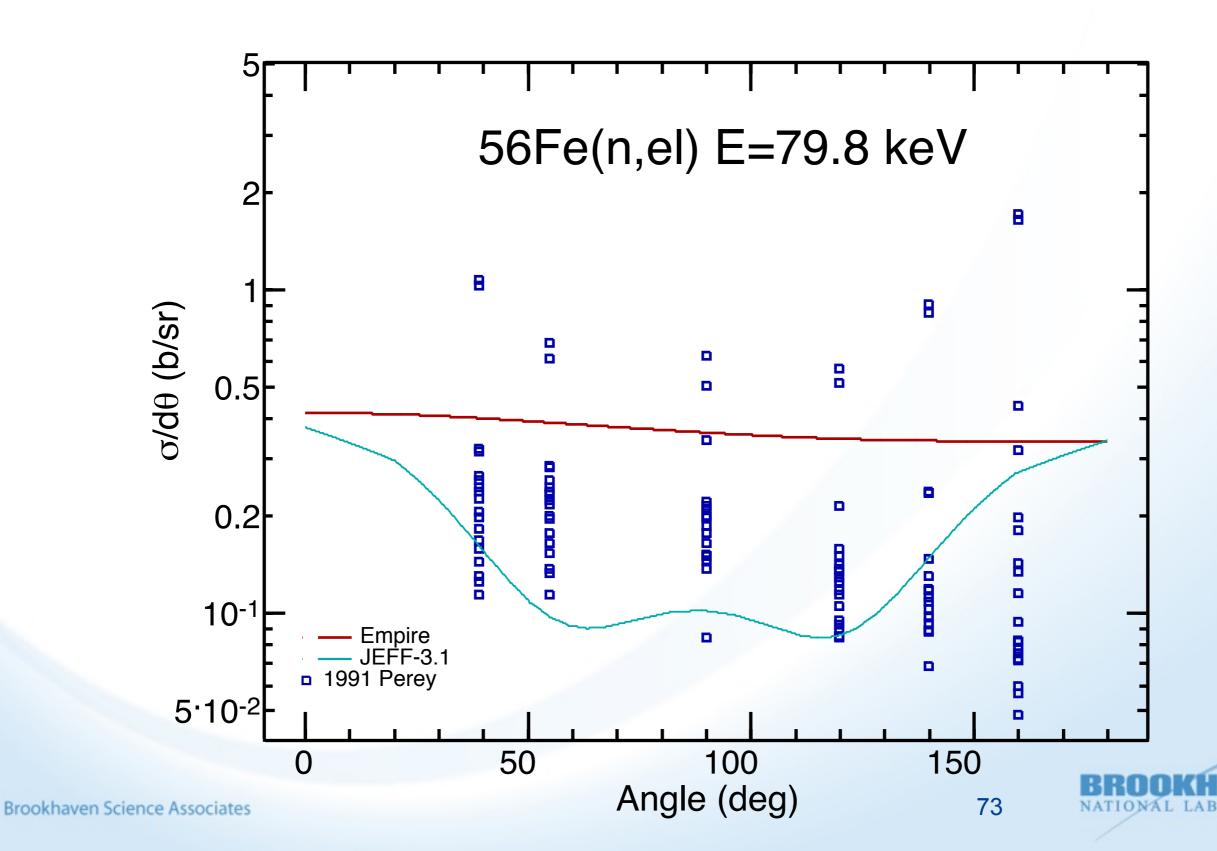


JEFF-3.1 <=> ENDF/B-VII.1 35 keV - 3.4 MeV (they usually differ, sometimes disagree)

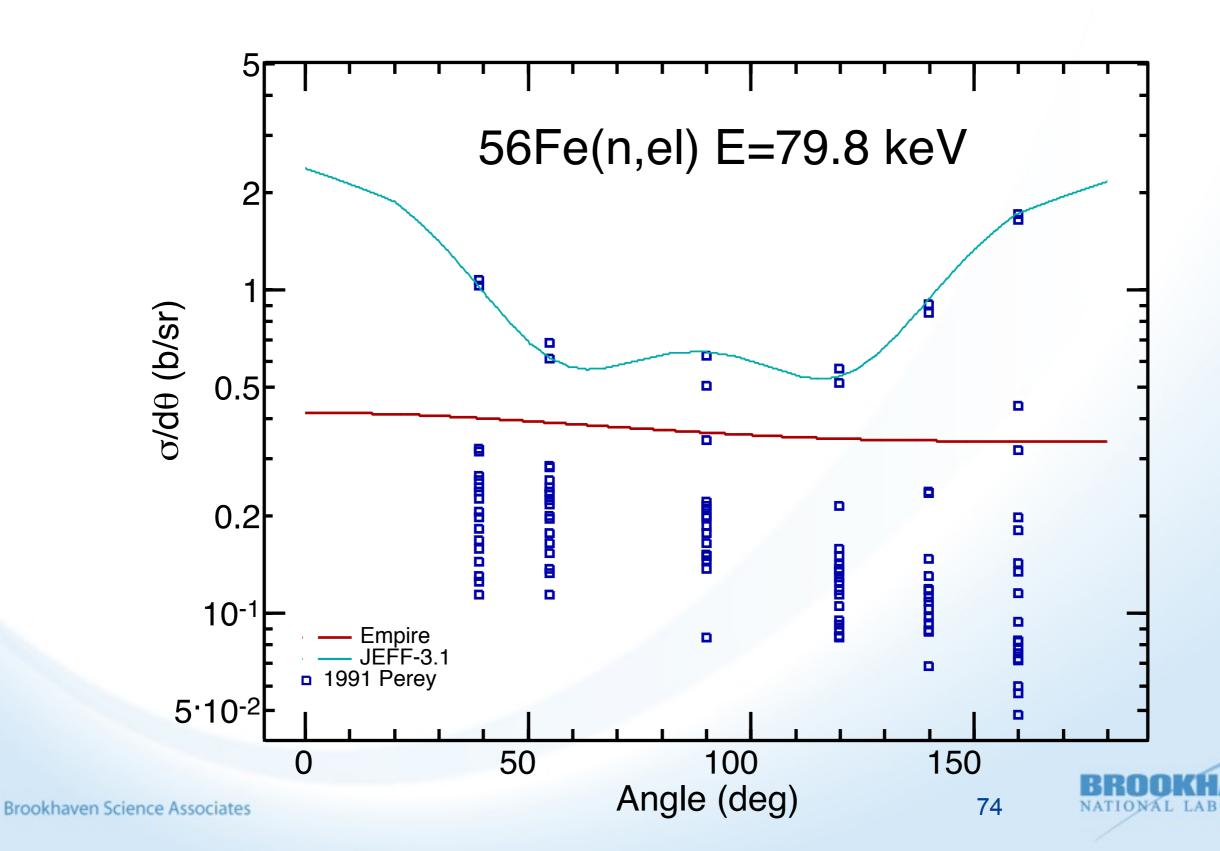
26-Fe-56(N,EL),DA Ei4.60E+6



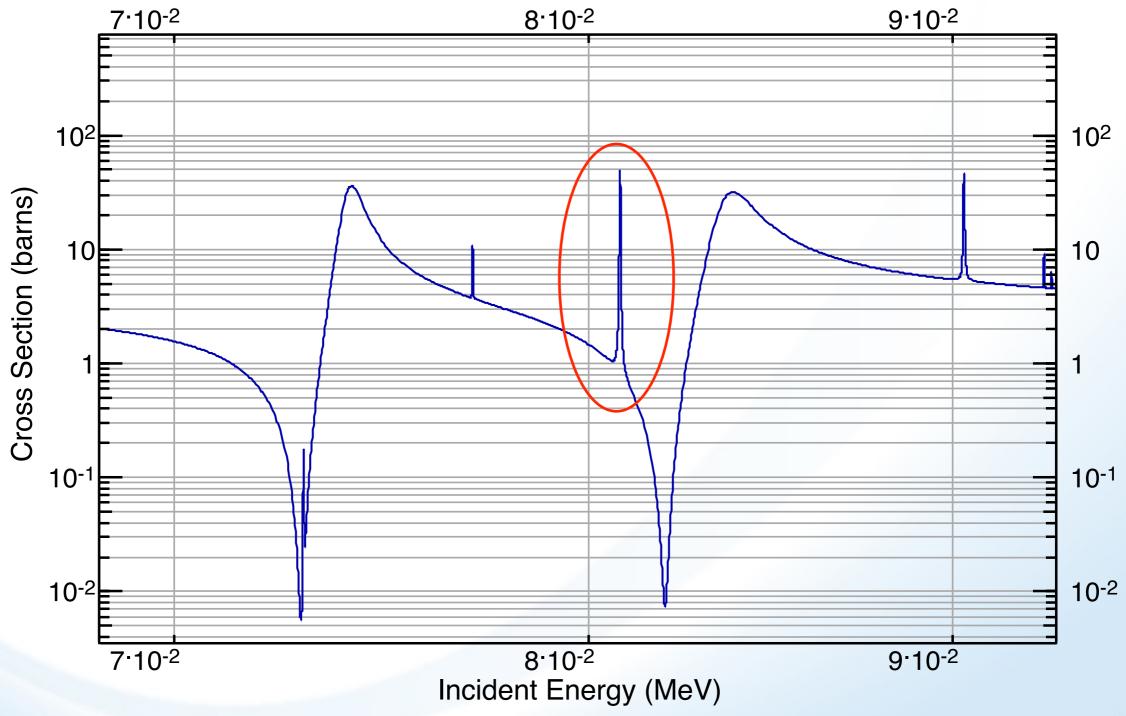
Compare with JEFF-3.1

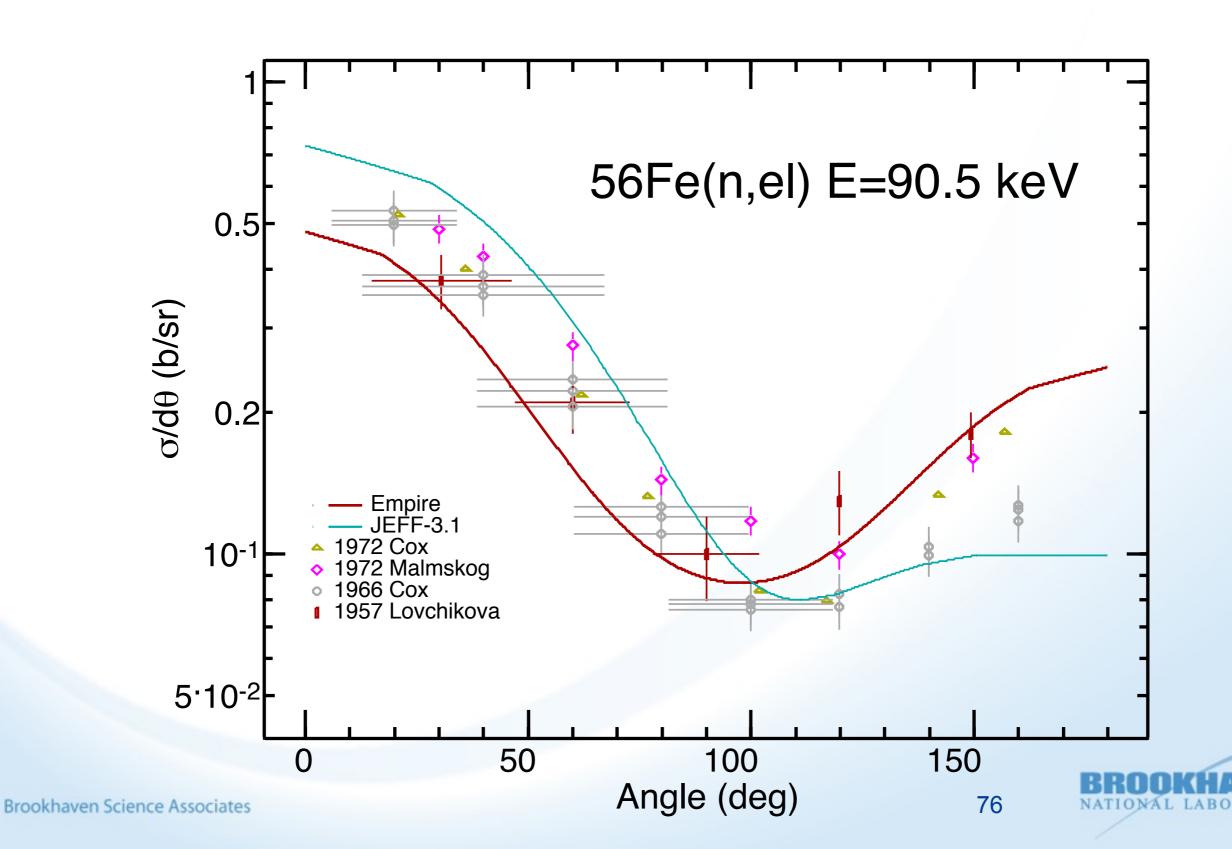


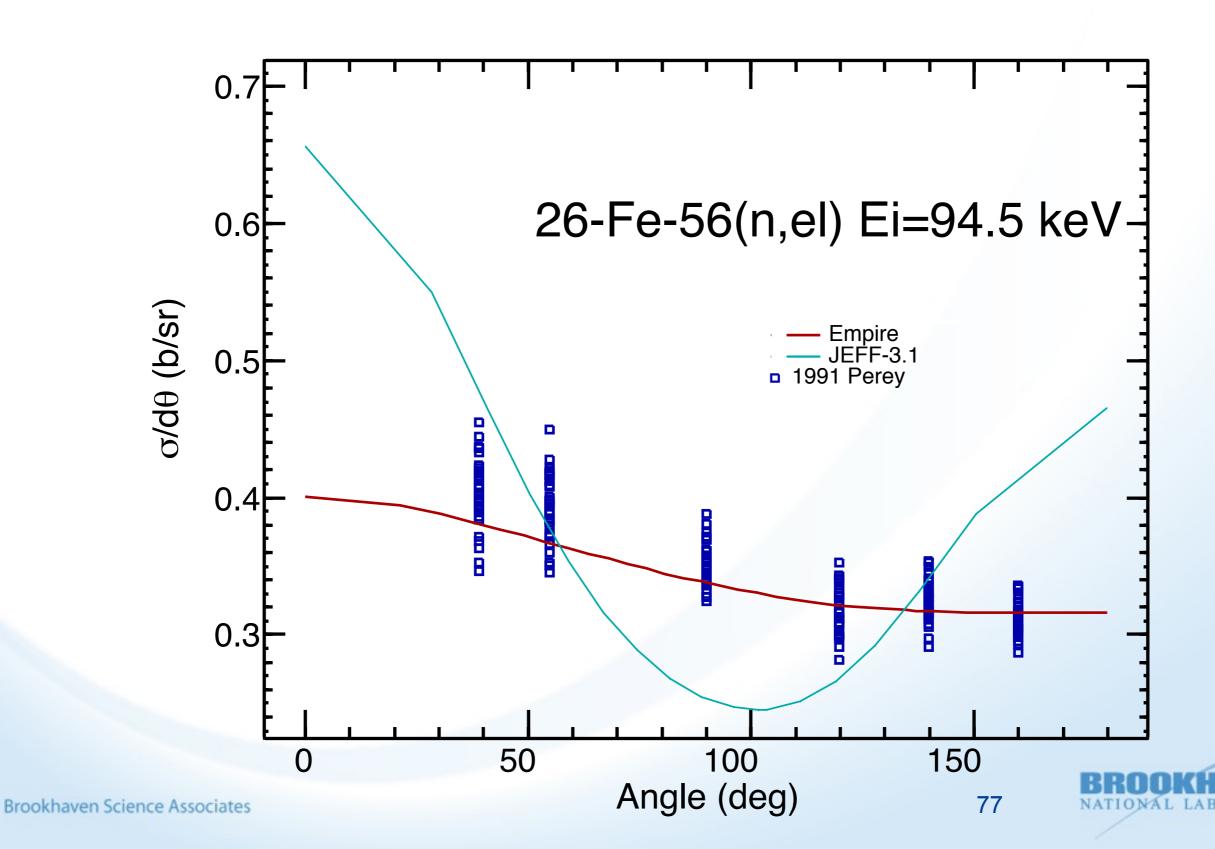
Shifting JEFF-3.1 up

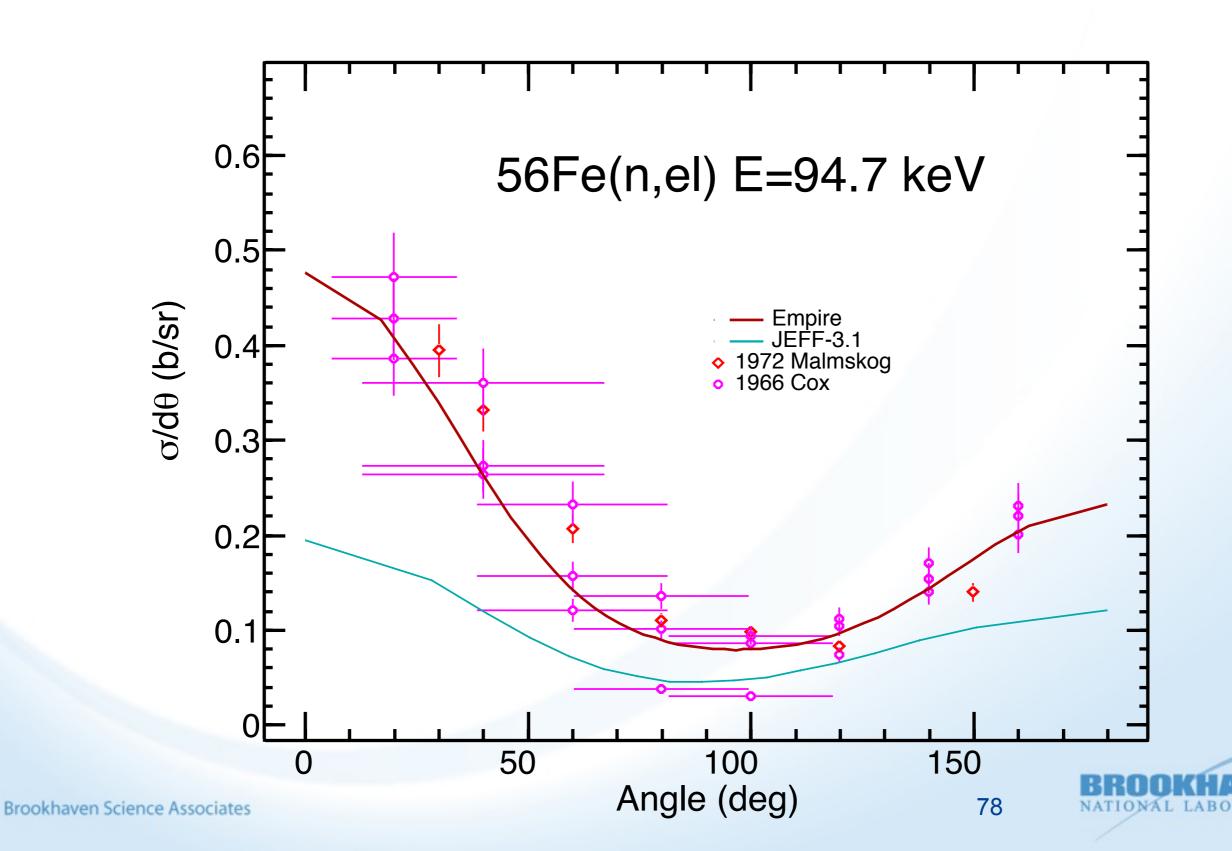


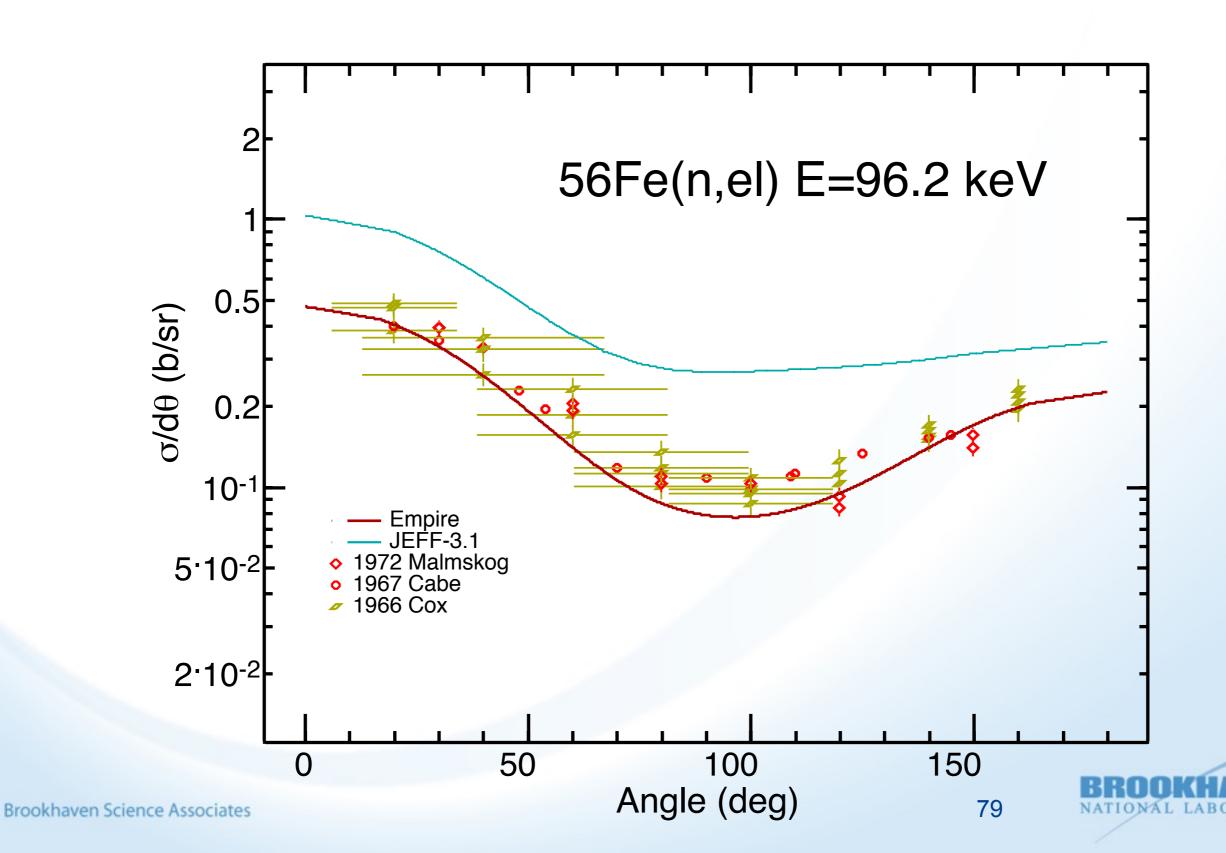
Resonance structure in ⁵⁶Fe around 80 keV

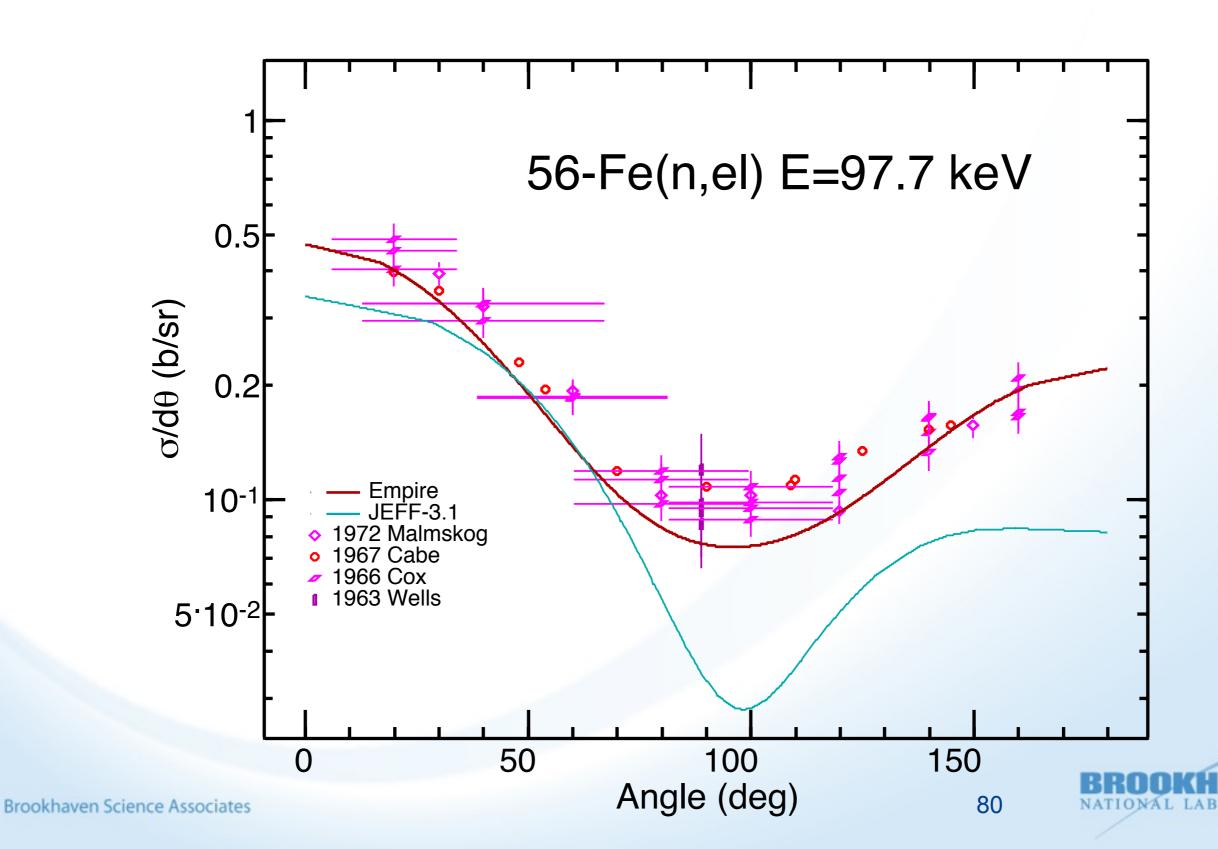


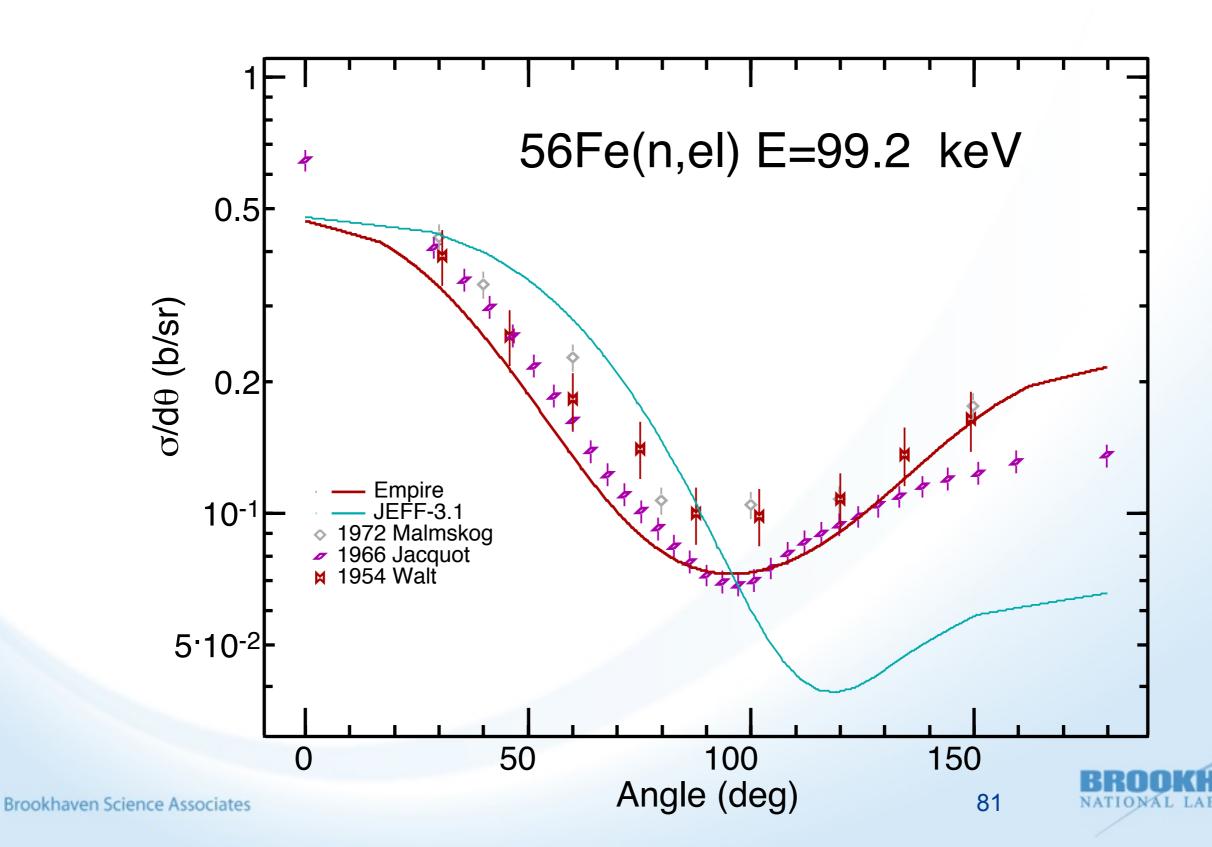


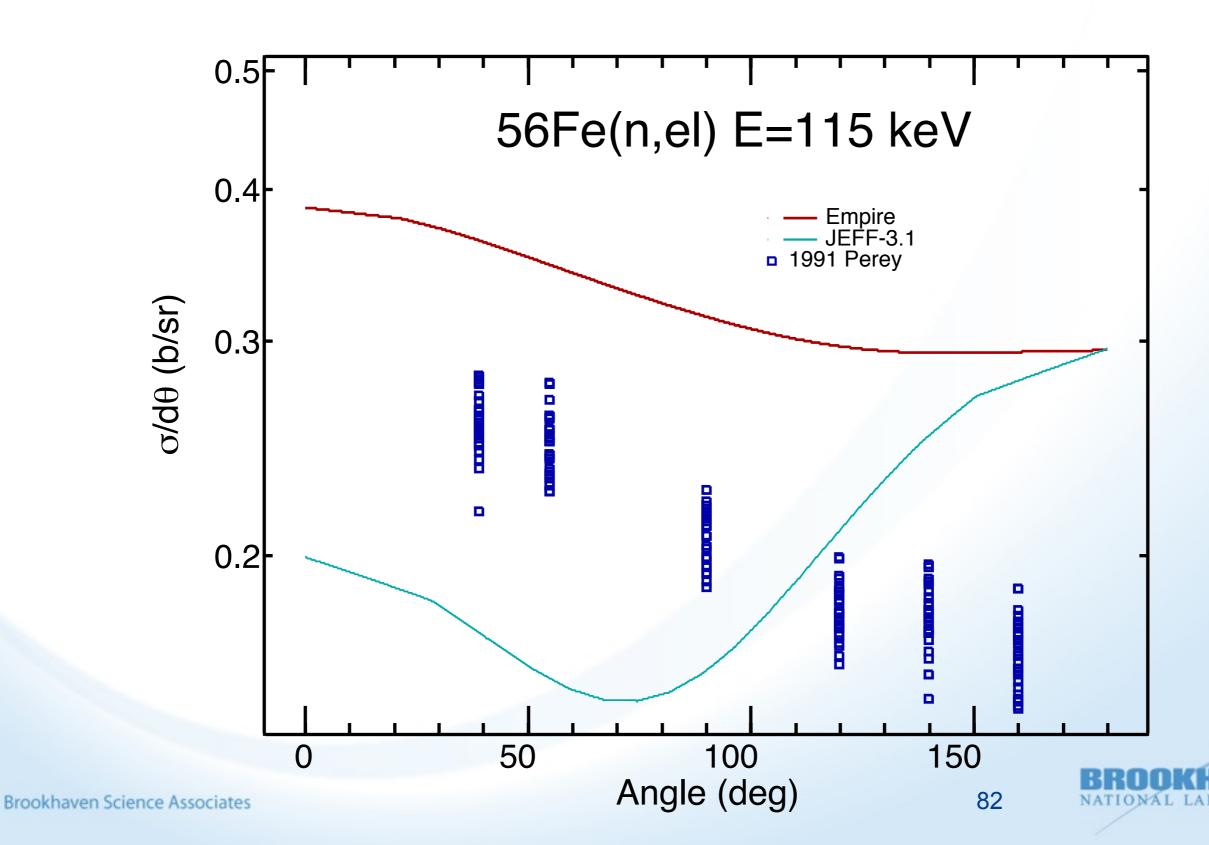


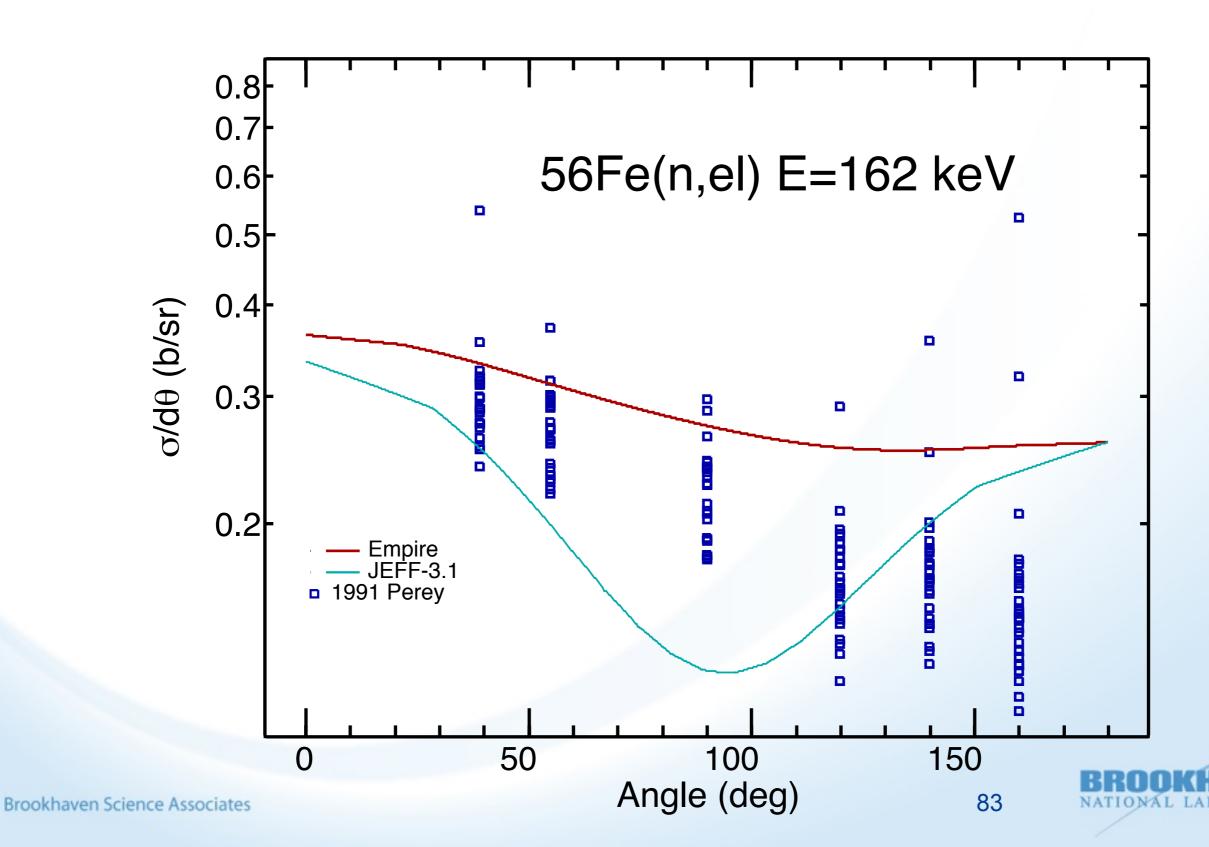




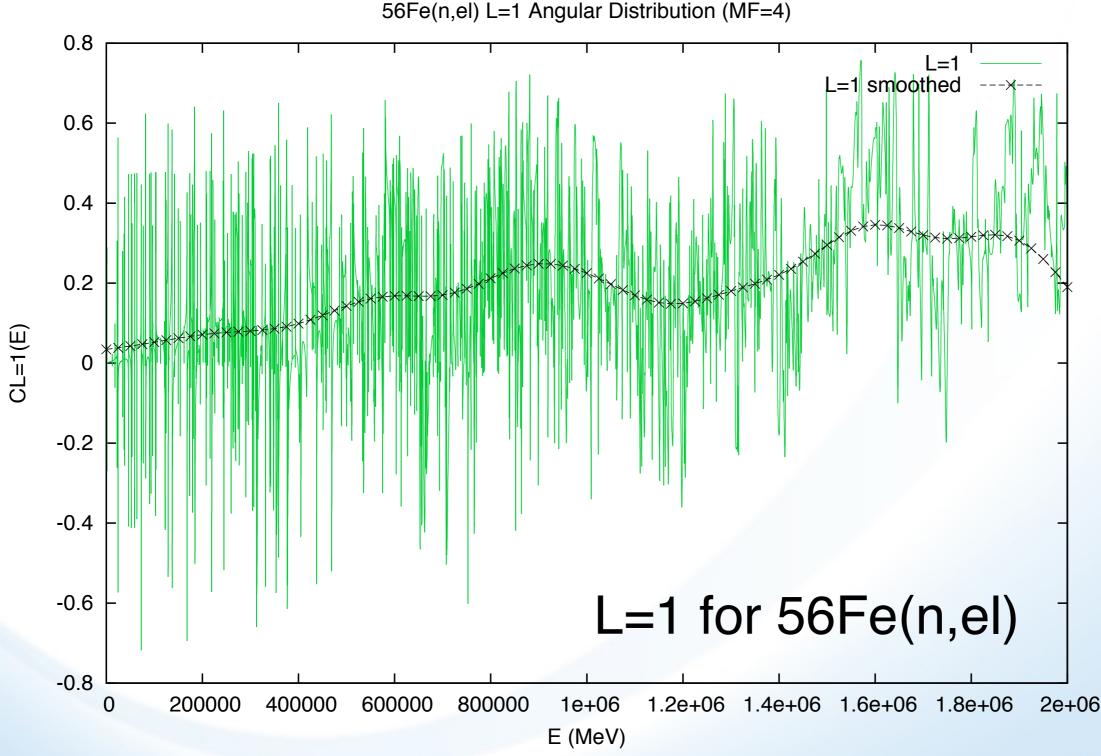


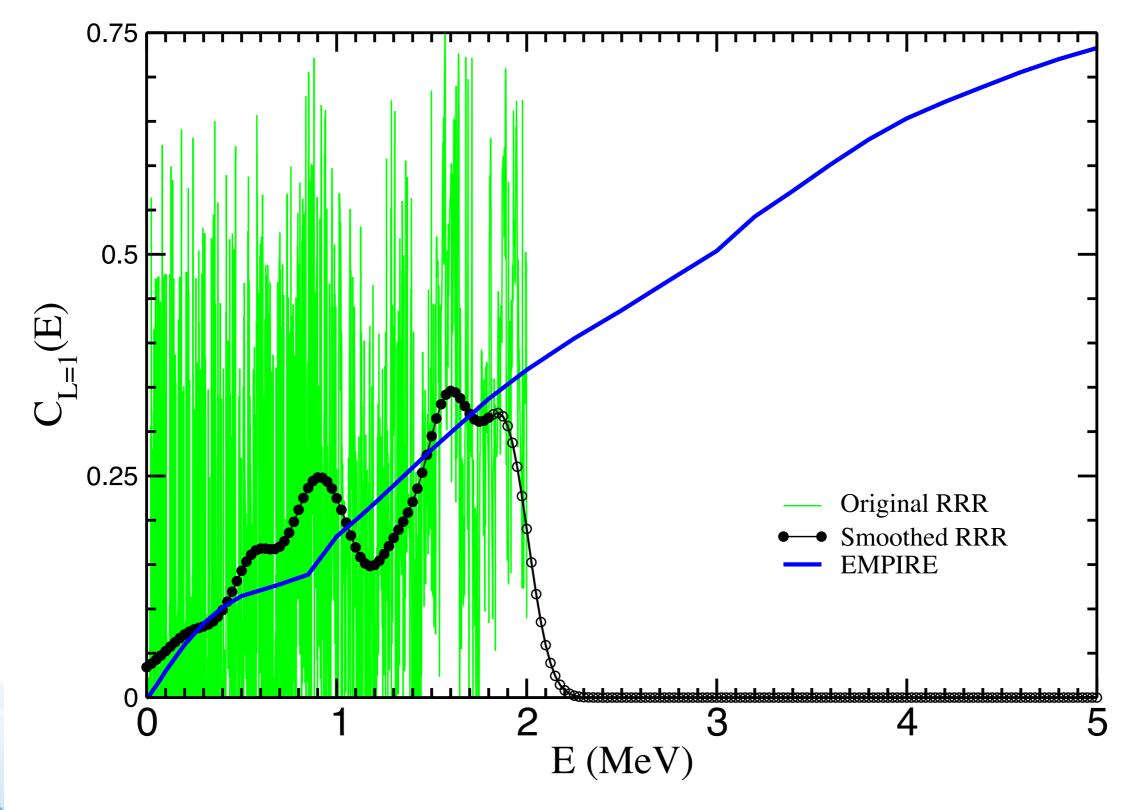




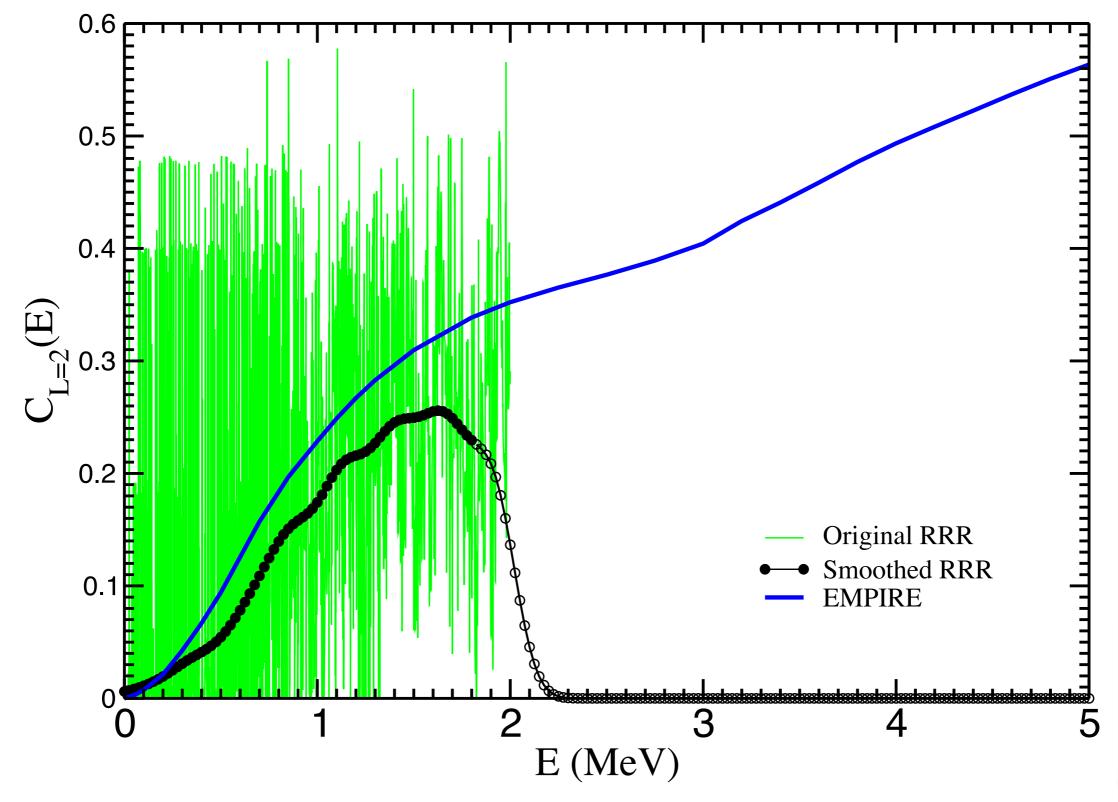


We smoothed the angular distribution one can reconstruct from RRR also

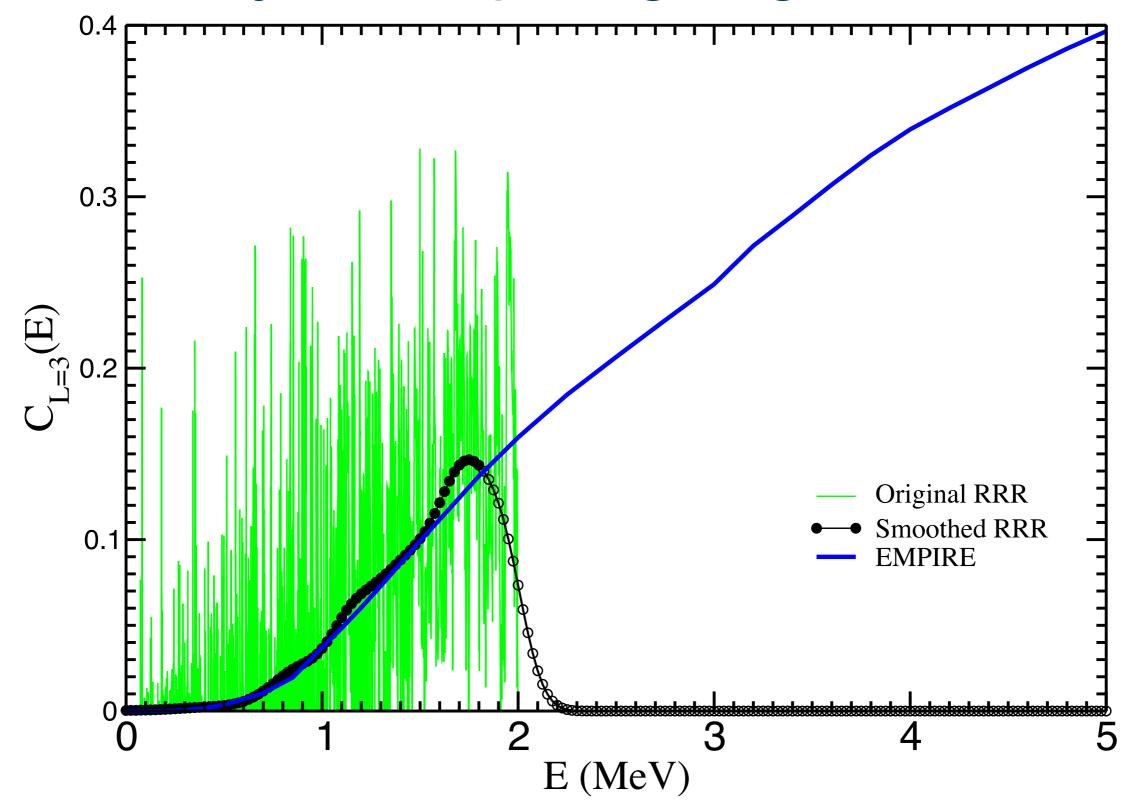




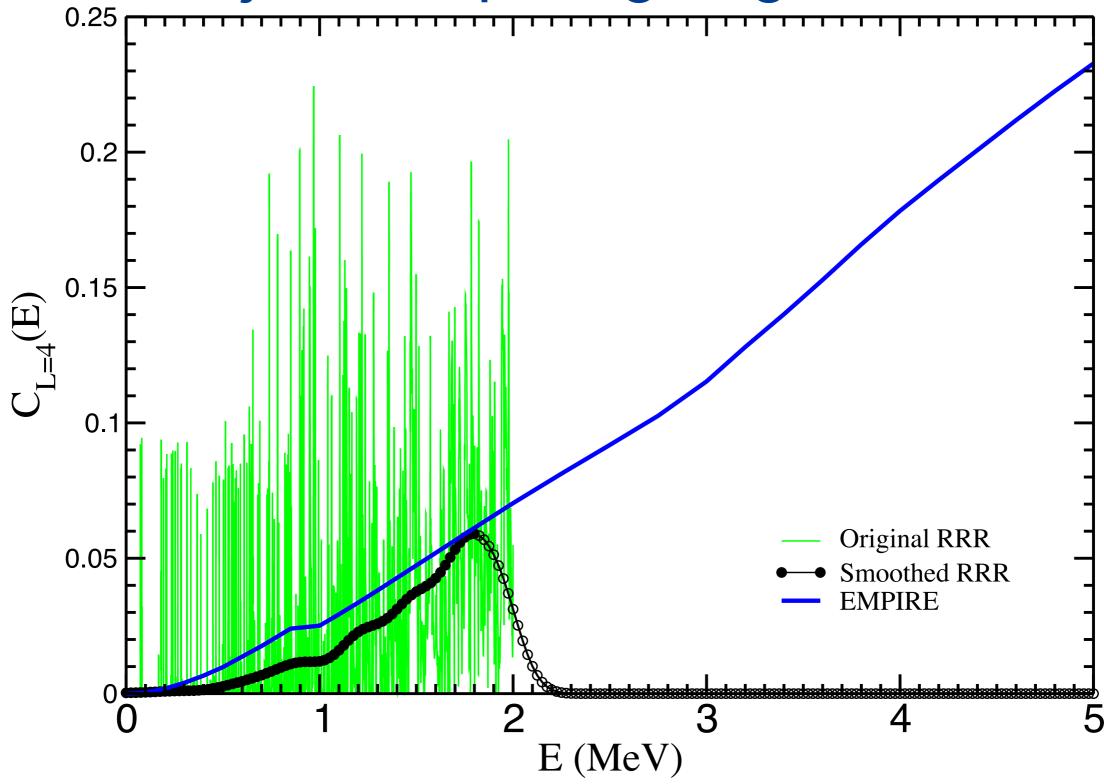




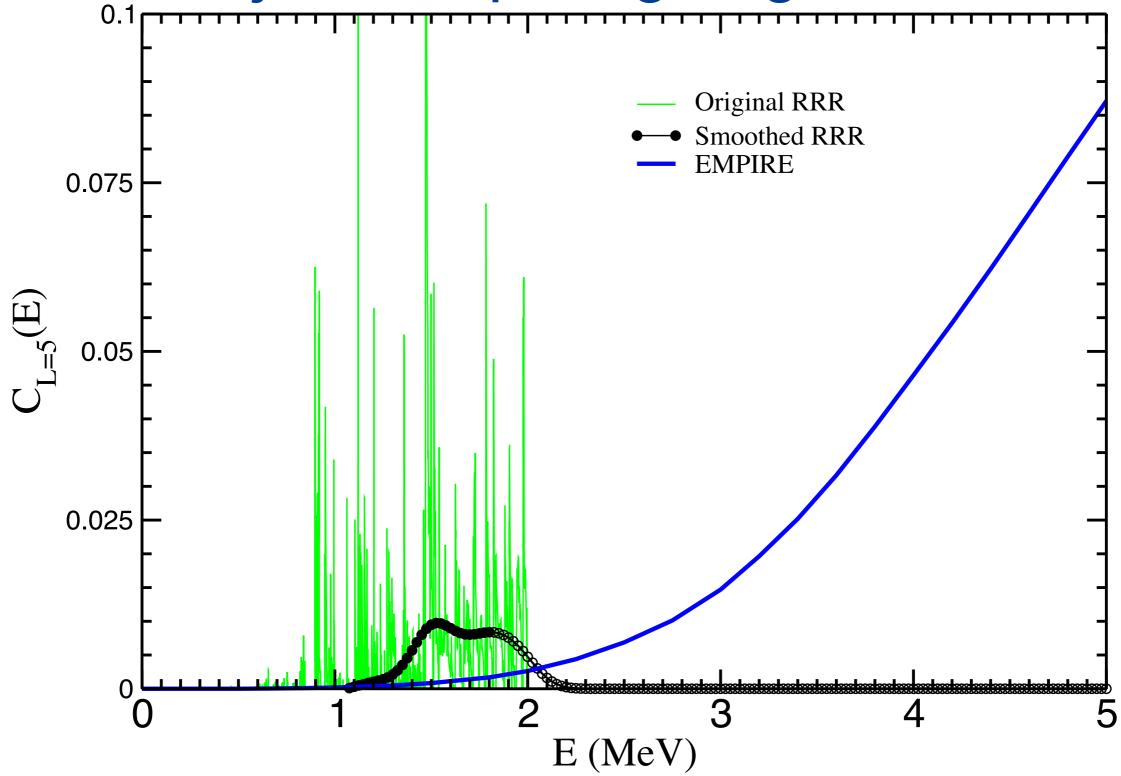




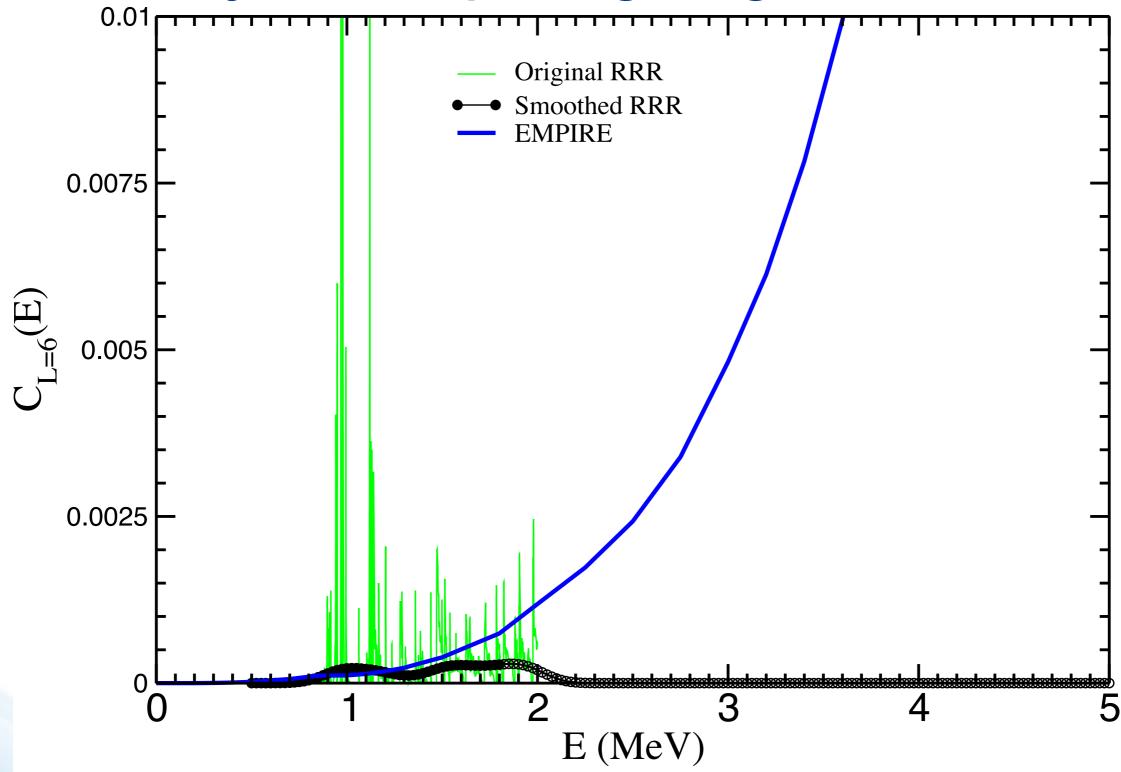














Along the way we have:

- solved mystery in the ENSDF/RIPL 56Fe level scheme
- discovered extraordinary sensitive monitor of level densities
- rediscovered Toshihiko's finding that OM for ⁵⁶Fe fails below 3
 MeV
- got a suspicion that angular distributions might be the key to the good iron evaluation
- realized the importance of having clean, differential data based, evaluation for being able to perform future updates



New data since 1995 (EFF-3.1 evaluation date)

- LANL (R. O. Nelson, M. Devlin, N. Fotiades, J. A. Becker, P. E. Garrett, W. Younes, D. Dashdorj, T. Ethvignot, T. Granier, AIP Conference Proceedings 819, 323 (2006); doi: 10.1063/1.2187879)
 - Found total inelastic (n,inel) by looking at main 847 keV line
- Geel (A. Negret, C. Borcea, Ph. Dessagne, M. Kerveno, A. Olacel, A. J. M. Plompen, M. Stanoiu, Phys. Rev. C 90, 034602 (2014))
 - Included (n,n₁') data in Leal's RRR fit
 - Backed out cross section data for first 10 excited states using coincidence gammas

Other new data:

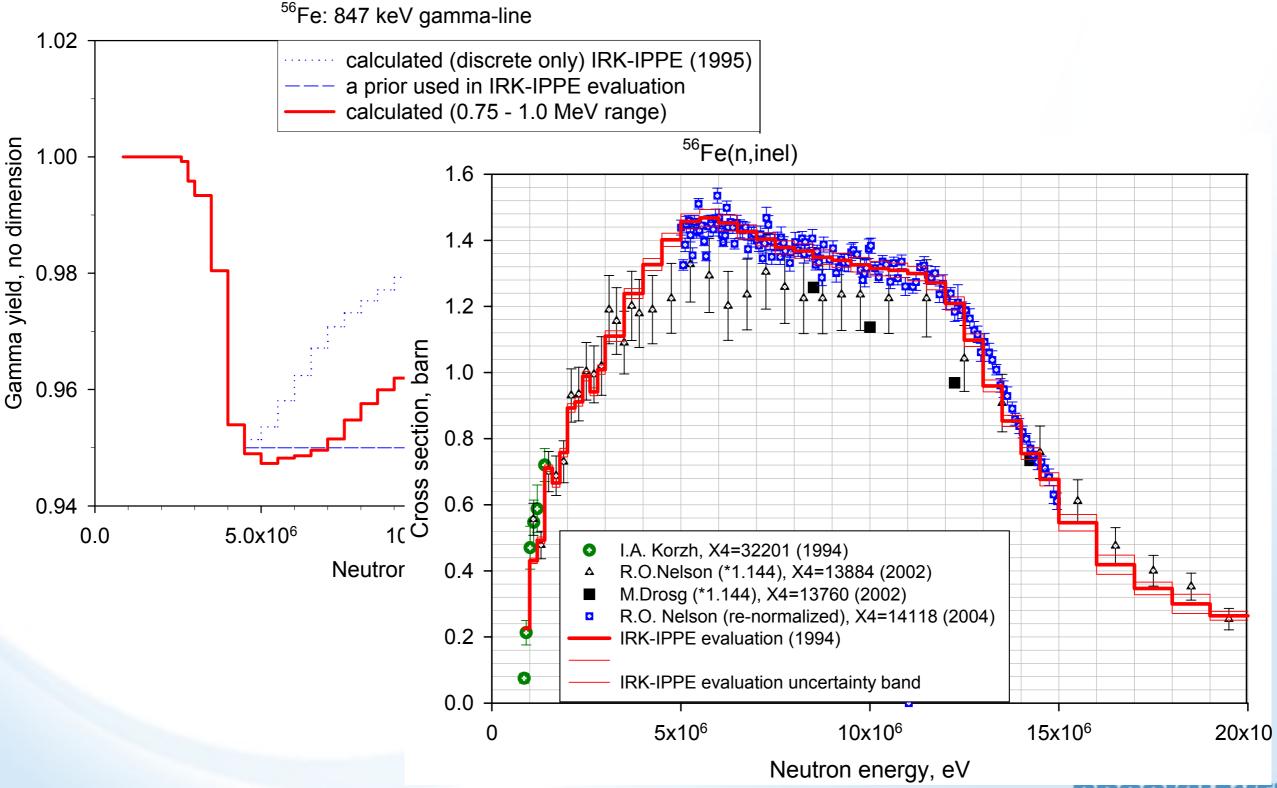
- RPI: quasi-differential data, good for validation
- Ohio U.: inelastic benchmarking, mentioned by Jing Qian already
- U. Kentucky: natFe inelastic cross sections, still being analyzed

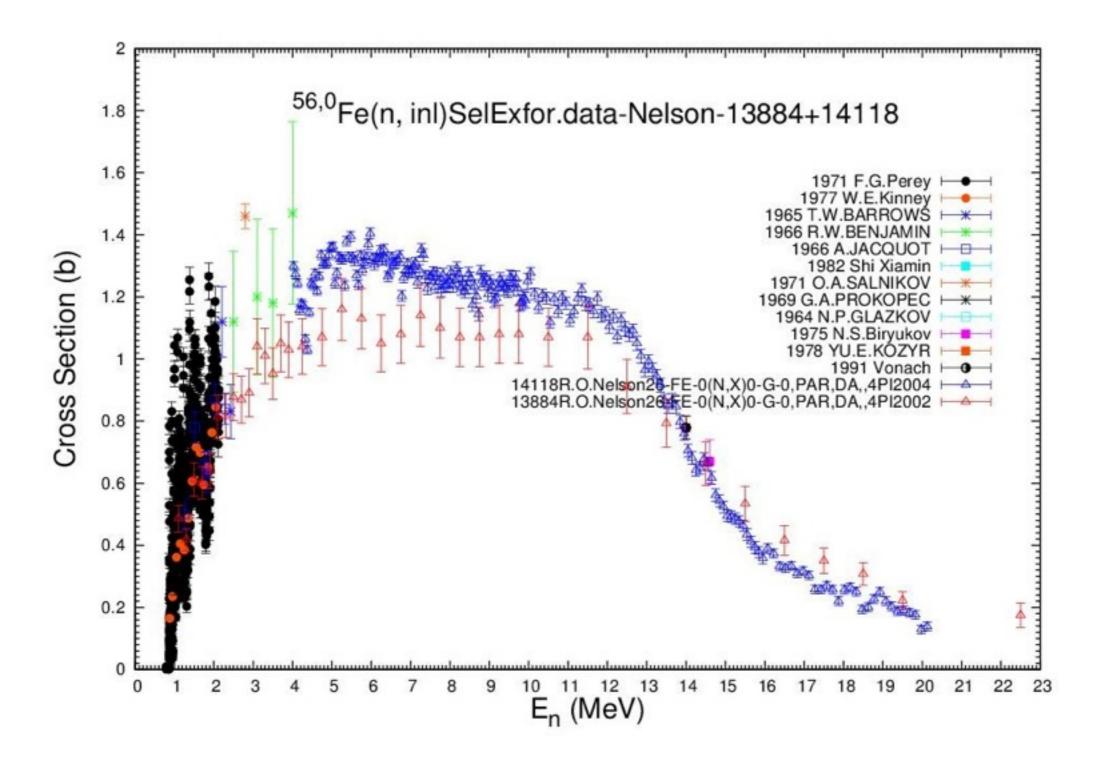


This is all almost ready for fitting

- Cross sections from EFF-3.1 evaluation
 - (n,2n)
 - (n,el) (Fast region)
 - (n,tot) (Fast region)
 - (n,p)
 - (n,a)
- Cross sections from CIELO RRR
 - (n,el) (RR region)
 - (n,g) (RR region)
 - (n,tot) (RR region)
- Inelastic cross sections from Geel
 - MT=52-60
- But... we still have mysteries to resolve

⁵⁶Fe(n,inel)

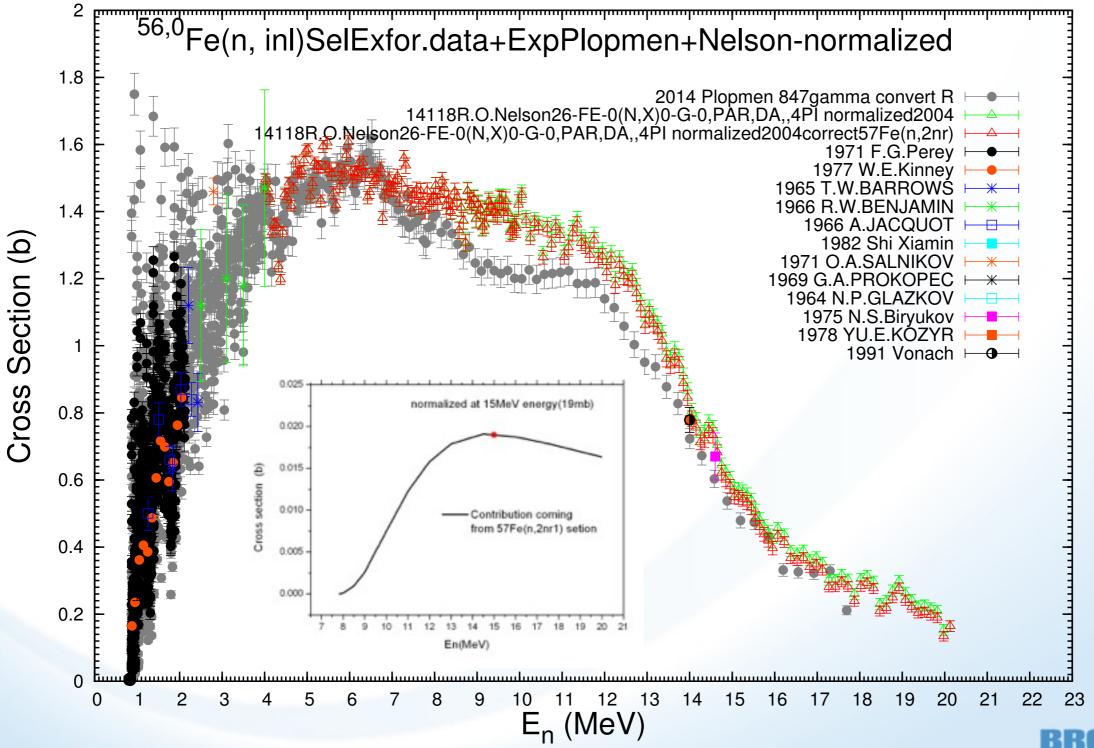






57Fe(n,2n) correction

Brookhaven Science Associates



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Path forward

- Implement IRK-IPPE evaluation into the fit
- Fully eliminate spooky level in ⁵⁶Fe from the calculations
- Decide on Geel-GEANIE controversy in inelastic >8 MeV
- Compare angular distributions derived from the resonance parameters with those obtained from optical model and decide on representation
- Perform fine tuning to differential data => ENDF/A
- Validate new file
- Perform adjustment to the integral data => ENDF/B ENDF/C

Still a lot of work but 'materials' and 'tools' are ready!

